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Coal Gasification/Gas Cleanup Test Facility Volume III. Environmental Assessment of Operation with New Mexico Subbituminous Coal and Chilled Methanol

North Carolina State Univ. at Raleigh

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COAL GASIFICATION/GAS CLEANUP TEST FACILITY: VOLUME III. ENVIRONMENTAL ASSESSMENT OF OPERATION WITH NEW MEXICO SUBBITUMINOUS COAL AND CHILLED METHANOL.

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16. ABSTRACT

The report concerns the second major study carried out on a pilot-scale coal gasification/gas cleaning test facility, namely, the steam-oxygen gasification of a New Mexico subbituminous coal using refrigerated methanol as the acid gas removal solvent. The report briefly describes the facility; summarizes gasifier operation using the New Mexico coal; gives results of mathematical modeling of the gasifier, detailed chemical analyses of gasifier effluent streams, and operation of the acid gas removal system using the gasifier make-gas as feed; and summarizes results of mathematical model development for the acid gas absorber column. Several trace sulfur compounds and aliphatic hydrocarbons were found to distribute among all exit streams from the acid gas removal system. In addition, a wide range of simple aromatic hydrocarbons were found to accumulate in the recirculated methanol.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS		b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group	
Pollution	Chemical Analysis	Pollution Coltrol	13B	07D
Coal Gasification		Stationary Sources	13H	
Gas Scrubbing		Methanols	07A	
Subbituminous Coal			21D	
Carbinols			07C	
Mathematical Models			12A	

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ABSTRACT

This report describes the results of the second major series of runs made using a pilot-scale coal gasification and gas cleaning facility located at North Carolina State University. These runs utilized a New Mexico subbituminous coal from the Navaho mine of the Utah International Co. as gasifier feed, and refrigerated methanol as the AGRS solvent. The pilot plant facility was described in detail in Volume I of this report series (Ferrell et al., 1980), and consists of a fluidized bed reactor, a cyclone and venturi scrubber for particulates, condensables, and solubles (PCS) removal, and absorption and stripping columns for acid gas removal and solvent regeneration.

A total of 15 gasification runs were made using the pilot plant facility with the New Mexico subbituminous coal. Six runs made use of the gasifier-PCS system only, and nine runs were integrated and included the acid gas removal system.

The most important quality assurance test for the evaluation of the experimental data was good closure on the mass balances for total mass and for all major elements. In general, the mass balance results for both the gasifier-PCS system and the acid gas removal system are excellent, and indicate that there are no gross errors in either chemical analyses or mass flow measurements.

The reactor temperature and steam-to-carbon feed ratio were the main operating parameters varied in the gasifier. Results show that the make gas flow rate and the carbon conversion both increase with increasing temperature. This is to be expected, as the degree of devolatilization and the gasification reaction rates all increase with increasing temperature.

In the gasification of New Mexico coal a large number of hydrocarbon gases are produced. Aliphatics up to butene and butane and simple aromatic compounds have been detected in the gasifier make gas stream. An analysis of these hydrocarbon emission rates indicates that they generally increase with increasing reactor bed temperature.

Analyses of the material condensed from the make gas stream indicate that a significant amount of PNA's, phenols, and other higher molecular weight hydrocarbons are in the gas stream as it leaves the reactor, and emerge primarily in the stream condensed by the venturi scrubber. It appears that compounds with boiling points higher than that of naphthalene are not

present in the gas stream past the PCS system.

A major effort was made to develop methods for the detection of trace metal elements in the feed and effluent streams, and to achieve closed mass balances on the elements arsenic, lead, and mercury. Analysis methods were generally satisfactory, but mass balance results on trace metals still leave much to be desired.

To aid in the formulation of gasifier performance correlations, a simple mathematical model of the fluidized bed gasifier has been developed which considers the gasification process to occur in three stages: instantaneous devolatilization of coal at the top of the fluidized bed, instantaneous combustion of carbon at the bottom of the bed, and steam/carbon gasification and water gas shift reaction in a single perfectly mixed isothermal stage. Using optimal parameter values, the model gave excellent predictions of carbon conversion, dry make gas flow rate, and the rate of evolution of individual species.

Results from the acid gas removal system show that refrigerated methanol is an effective solvent for cleaning of gases produced by coal gasification. The removal of CO_2, COS, and H_2S to sufficiently low levels can be achieved with proper choice of operating conditions and effective solvent regeneration.

The presence of several trace sulfur compounds, mercaptans, thiophenes, organic sulfides, and CS_2, complicates the gas cleaning process. These compounds were found to distribute among all exit streams from the AGRS.

A wide variety of aliphatic and aromatic hydrocarbons were present in the gas stream fed to the AGRS. The aliphatic hydrocarbons, ranging from methane to butane, cover a wide range of solubilities. Their presence in all AGRS streams must be anticipated to prevent their emission to the atmosphere.

While a wide range of simple aromatics were identified in the gas stream fed to the AGRS, essentially no polynuclear aromatic compounds were found. The gas quenching process effectively removes these compounds from the gasifier product gas. However, significant quantities of simple aromatics were found to accumulate in the recirculating methanol increasing the potential for their discharge to the atmosphere.

As a part of the AGRS research program, a mathematical model of the absorber was developed and showed excellent agreement with measured absorber column temperatures and with measured absorber concentrations for most compounds.

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INTRODUCTION

As a part of a continuing research program on the environmental aspects of fuel conversion, the U. S. Environmental Protection Agency has sponsored a research project on coal gasification at North Carolina State University in the Department of Chemical Engineering. The facility used for this research is a small coal gasification-gas cleaning pilot plant. The overall objective of the project is to characterize the gaseous and condensed phase emissions from the gasification-gas cleaning process, and to determine how emission rates of various pollutants depend on adjustable process parameters.

A complete description of the facility and operating procedures is given by Ferrell et al., Vol I, (1980), and in abbreviated form by Felder et al. (1980). A schematic diagram of the gasifier, the acid gas removal system (AGRS), and other major components is shown in Figure 1, and a brief description of the facility is given in a later section of this report.

In an initial series of runs on the gasifier, a pretreated Western Kentucky No. 11 coal was gasified with steam and oxygen. The results of this work and a detailed listing of the project objectives are given by Ferrell et al., Vol II, (1981), and were presented at the EPA Symposium on Environmental Aspects of Fuel Conversion Technology V, held in St. Louis, Mo., September, 1980.

This report concerns the second major study carried out on the facility, the steam-oxygen gasification of a New Mexico subbituminous coal using refrigerated methanol as the AGRS solvent. This coal was obtained from the Navaho mine of the Utah International Co., and was ground and screened by the Morgantown Energy Technology Center of the Department of Energy. Table 1 shows an average analysis of the char and coal used in studies to date.

This report presents a brief description of the facility, a summary of the gasifier operation using the New Mexico coal, the results of mathematical modeling of the gasifier, the results of detailed chemical analyses of gasifier effluent streams, the results of the operation of the AGRS using the gasifier make gas as feed, and a summary of the results of mathematical model development for the AGRS absorber.

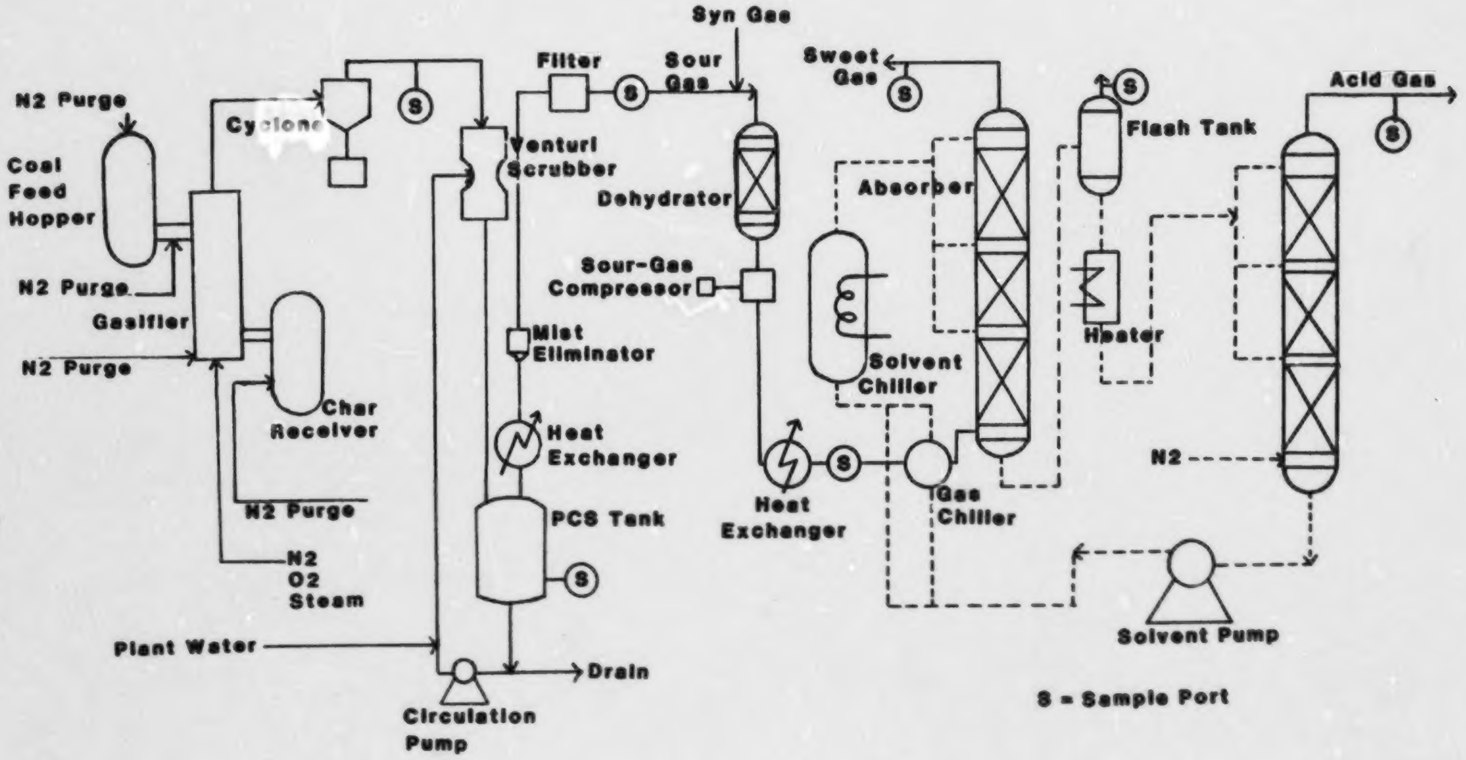

N2 Purge
Coal Feed Hopper
N2 Purge
Gasifier
N2 Purge
Cyclone
Char Receiver
N2 Purge
N2
O2
Steam
Plant Water
S
Venturi Scrubber
Circulation Pump
Mist Eliminator
Heat Exchanger
PCS Tank
S
Drain
Filter
S
Sour Gas
Syn Gas
Dehydrator
Sour-Gas Compressor
Heat Exchanger
S
Sweet Gas
S
Absorber
Solvent Chiller
Gas Chiller
S
Flash Tank
Heater
Acid Gas
S
N2
Solvent Pump
S = Sample Port

Figure 1

Pilot Plant Facility

TABLE 1
COAL AND CHAR ANALYSIS

	Coal Char wt %	New Mexico Coal wt %
Proximate Analysis		
Fixed Carbon	86.0	36.2
Volatile Matter	2.4	31.1
Moisture	0.9	9.7
Ash	10.7	23.0
Ultimate Analysis		
Carbon	83.8	50.2
Hydrogen	0.6	4.2
Oxygen	2.2	20.7
Nitrogen	0.1	1.1
Sulfur	2.6	0.8
Ash	10.7	23.0

THE FACILITY

The pilot plant facility is a small but complete coal gasification - gas cleaning plant. The plant is capable of achieving long periods of steady operation, and can therefore produce a full set of product and effluent streams under known and steady conditions. Measurement of flow rates and compositions of these streams under such conditions gives a true measure of product gas composition and production rates, and a good evaluation of environmental problems.

The principal components of the pilot plant are a continuous fluidized bed gasifier, a cyclone separator, a venturi scrubber, and an acid gas removal system. A process control and data acquisition system for operation, data logging, and display is also used. Each of these systems is described briefly in the following sections:

THE GASIFIER

The gasifier is a fluidized bed reactor consisting of a 15.2 cm (6 in) I.D. Schedule 40 pipe (316 SS) enclosed in several layers of insulation and contained in a 61 cm (24 in) I.D. Schedule 80 carbon steel pipe. The overall height of the reactor is about 3.7 m (12 ft) of which 3 feet is used as a reaction zone. Three triangularly arranged nozzles are used to feed steam, nitrogen, and oxygen into the reactor which normally operates near 790 kPa (114.7 psia). Thermocouples are mounted in the center of the bed above the gas distributing nozzles to monitor the bed temperature profile.

Coal is fed and spent char is removed from the reactor by screw conveyors from pressurized hoppers at either end of the reactor. A nuclear level gauge is used to monitor the fluidized bed height, which is controlled by adjusting the char removal rate. The operating temperature normally ranges from 870 to 1040 °C (1600 to 1900 °F).

THE PCS SYSTEM

Gas exiting the gasifier contains particulates, tars, and heavy oils as well as several water-soluble compounds which are removed in the PCS system (PCS stands for particulates, condensables, and solubles). A cyclone separator collects entrained particulates and a venturi scrubber is used to quench the gas to remove condensables and water-soluble compounds. Heat exchangers reduce the temperature of the quenched gas stream to near room temperature. Either fresh city water or water recycled from the scrub water tank can be fed to the venturi scrubber. Finally, a mist eliminator, a series of filters, and a dehydrator remove the last traces of particulates and water before the gas is fed to the acid gas removal system.

A Western Kentucky No. 11 coal char, containing only trace amounts of volatile matter, was gasified in the early stages of operation. The gas produced from this feedstock was relatively free of tars and oils. Initial work with the higher volatile matter New Mexico sub-bituminous coal led to the production of considerable amounts of tar and forced the shutdown of operation due to line pluggage.

The PCS system was reconstructed by increasing the size of the line leaving the gasifier from one inch to three inches in diameter. The venturi scrubber was replaced with a series of spray nozzles at the inlet of the scrub water tank. At this point in the system the pipe size is reduced from three inches to one inch to promote better gas-liquid contacting. A heat exchanger, used previously to cool the gases downstream of the venturi scrubber, was removed and cooling coils were installed inside the scrub water tank to keep the water temperature well below the boiling point. A water separator was also installed downstream of the outlet heat exchanger to remove any entrained water in the exiting gas stream. In addition, the top of the gasifier reactor vessel was rebuilt to enlarge the coal feed and the gas exit lines.

The modified system has functioned well in providing a clean, dry gas to the acid gas removal system.

THE ACID GAS REMOVAL SYSTEM

The major purpose of the acid gas removal system (AGRS) is to remove carbon dioxide and hydrogen sulfide from the product gas stream. In so doing it also usually removes all of the other sulfur gases and many of the hydrocarbons of molecular weight higher than methane.

The acid gas removal system used in this study is modular in design so that alternative absorption processes can be evaluated. The system was designed to operate with four different solvents: refrigerated methanol, hot potassium carbonate, monoethanolamine, and the dimethyl ether of polyethylene glycol. With minor modifications, other solvents could also be used. Refrigerated methanol has been used so far in this study.

The major components of the AGRS are an absorption column, a flash tank, and a stripping column with the necessary auxiliary equipment. Gases from either the gasifier or gas cylinders are fed to the system through a pair of dehydrating towers containing molecular sieves. The gases are compressed to a pressure ranging from 1825-3200 kPa (250-450 psig) in a two-stage compressor and then cooled to remove the heat of compression. These gases are cooled further in a chiller by exchange with cold solvent leaving the stripper bottom. They are then fed to the absorber at a point just below the packing support to minimize end effects.

The absorption column contains three 2.2 m (7.1 ft) sections of 6.4 mm (1/4") ceramic Intalox saddle packing. The column is well-insulated and approaches adiabatic operation. Solvent which is cooled in a refrigeration unit can be fed to the absorber at the top of the first, second, or third packed section. This provides flexibility in mass transfer studies.

The solvent exiting the absorber is fed to a flash tank where some of the absorbed gases are released. The solvent then exchanges heat with the solvent exiting the stripper and is fed to the stripper. The stripper is similar to the absorber in design in that it contains three packed sections of ceramic Intalox saddles, any or all of which sections can be used in mass transfer studies. The column approaches adiabatic operation, and the solvent can be regenerated either by stripping with an inert gas or with the reboiled methanol vapors.

For more carefully controlled mass transfer studies, a synthetic gas feed stream (SYNGAS) can be prepared at a mixing manifold. Any or all of the gases produced in the gasifier can be fed to the AGRS. Most of the SYNGAS runs made in this study used a mixture of nitrogen and carbon dioxide as the feed gas to evaluate packing characteristics and to determine the heat of solution of carbon dioxide in methanol.

PROCESS CONTROL AND DATA ACQUISITION SYSTEM

Approximately 100 process sensors are used to obtain information during pilot plant operation. The process is controlled with a Honeywell TDC 2000 process control computer which has a capability of regulating 16 process control loops throughout the pilot plant. Also, an alarm system incorporating all process sensors calls attention to process problems by sounding an audible alarm and lighting an alarm light on a process schematic above the control panel. The alarm system can also be set to cause plant shutdown automatically for pre-set alarm points.

The 100 process sensors (temperatures, pressures, differential pressures, flow rates, and levels) are monitored through a data acquisition system linked to a PDP 11/34 minicomputer. Each sensor is interpreted every five seconds for display on a video terminal. The information is averaged and stored every five minutes on magnetic disk for future data reduction. The capability to plot information from each process sensor for the previous hour on a video or hard-copy terminal during the run also exists. Strip chart recorders are used for continuous monitoring of process temperatures and selected process variables.

The data acquisition computer system is also used for all data reduction calculations and is programmed to produce output results in a form suitable for reports. Examples are given later in this report.

DESCRIPTION OF PROCESS STREAMS AND SAMPLING PROCEDURES

This section presents a brief description of the various effluent and process streams, and how they were metered, controlled, sampled, and analyzed. Most of the input and output stream sample points are shown on Figure 1. The sample train, mentioned frequently in the sections that follow, is located just downstream of the cyclone.

INPUT STREAMS

Coal Feed

Multiple samples of the feed coal were taken before each run, sieved, subjected to proximate and ultimate analyses, and analyzed for several trace elements. The analytical methods used for trace metal analysis will be described later in this section. For several runs, elemental analyses were made for all sieve sizes.

The coal feed stream was metered into the reactor by controlling the rate of revolution of the feed screw. The quantity of coal delivered per revolution of the screw was fairly constant for these runs, and thus the coal feed rate during the steady state portion of a run could be determined accurately.

Gas Feeds

Gasifier Feed--

The oxygen feed was from a bank of six cylinders; the nitrogen feed was from a six-thousand gallon liquid nitrogen tank with an atmospheric vaporizer; and the steam feed was from a 150 psig building process steam line. All feed streams were preheated and metered, and were controlled by the process control computer system. The calibrations of the flow elements and transmitters were checked frequently during this experimental program.

AGRS Feed--

The gas feed to the AGRS was either a mixture of gases from cylinders or the gasifier make gas. In either case, the feed gas passed through a dehydration tower packed with molecular sieves, was compressed to approximately 50 Atm, and cooled to ambient temperature. The desired flow rate to the absorber was controlled and measured by an orifice meter, calibrated at operating pressure.

OUTPUT STREAMS

Spent Char

Multiple samples were taken from the char receiver vessel or from the bottom of the reactor after a run. For some runs, especially when the carbon conversion was high and very little spent char was formed, some difficulty was experienced in obtaining a reliable sample representing the steady state portion of a run. Analyses were essentially identical to those for the feed coal. The steady state char removal rate was determined from the total char removed, the total revolutions of the removal screw, and the rate of revolution of the screw during the steady state. Char removal rates could be determined with much less reliability than coal feed rates due to the erratic performance of the removal screw.

Cyclone Fines

Samples were collected from the cyclone solids collection tank. Since the cyclone fines were sometimes slightly damp, it is possible that some condensation on the fines occurred during or after shutdown. Analytical methods were the same as those for the feed coal.

Condensed Phases After Venturi Scrubber (PCS Tank)

After shutdown, samples of particulates, tar, and water were taken from the PCS tank. For all runs reported on here, the venturi scrubber water was recirculated from the tank to the spray nozzles, and thus contains material from the startup, steady state, and shutdown periods. Prior to each run, the tank was filled with approximately 160 gallons of fresh water, and thus the final composition of the water depended on the length of the run. Methods of analysis and results are presented later in this report.

Gas Samples

Gas samples were taken from the six locations noted on Figure 1 at operating pressure using one liter stainless steel bombs, and at lower pressures using one liter glass bombs. The glass bombs were coated internally with hexamethyldisilizane to reduce the adsorption of trace sulfur, nitrogen and hydrogen species. For the purposes of sampling, the steady state period was determined by the stability of various temperatures, pressures, flow rates, and levels over long periods of time. Examples of plots of several critical process variables versus time are given in a later section of this report. Times at which samples were taken for the run shown are noted on the plots.

Gas Samples from the PCS System--

Gases from the PCS system were metered and sampled after the final filter and before the dehydrators. Samples were collected at high pressure in stainless steel bombs, and at a lower pressure (approximately 20 psig) in glass bombs for later analysis by gas chromatography. Analysis methods and results are presented later.

The reactor make gas flow meter-transmitter calibration was checked frequently, and the mass flow rate indicated by the data acquisition system was corrected for gas composition before being used for mass balances.

Gas Samples from the AGRS--

The gas sampling locations used for the AGRS are shown in Figure 1, and samples were taken as described above.

In the early phases of plant operation, it was noted that the oscillations introduced by process controller action made it difficult to obtain representative gas samples during steady state. To avoid this problem, manual control was used for certain process variables during sampling periods. All process controllers were, however, used for each controlled variable during the start-up and early part of the steady state period as well as during shutdown.

The most severe case of controller action problems involved the level controllers in the absorber and flash tank. As the absorber level controller cycled, it caused an oscillating liquid flow rate to the flash tank. Because the amount of gas released in the flash tank is proportional to the liquid flow to the tank, any sample of the flash tank exit gas taken at a particular time may not be representative of the steady state. The same problem occurs as the flash tank level controller cycles and delivers an oscillating liquid flow rate to the stripper.

Several attempts were made to tune process control loops to avoid this problem, but none proved entirely satisfactory. To remedy this problem, the absorber and the flash tank level controllers were put into manual control prior to sampling, and the valve position adjusted to allow only long term variations in liquid level. This practice proved to be successful, and resulted in satisfactory samples and mass balances.

The flow meter-transmitter calibrations at the absorber, flash tank, and stripper were checked frequently, and the mass flow rates indicated by the data acquisition system were corrected for gas composition before being used for mass balances.

Liquids

Water samples were taken from the PCS tank and the sample train and will be discussed in some detail in a later section of this report.

In the AGRS, liquid samples were taken at the exit line from the absorber, flash tank, and stripper at system pressure. These samples were then vaporized and injected into a gas chromatograph for analysis. Attempts to take samples from the column packing were unsuccessful due to problems of liquid entrainment and flashing.

Sample Train

In addition to the normal effluent streams, a small side stream was drawn off just downstream of the cyclone and passed through a sample train. A schematic diagram of the sample train is shown in Figure 2. For mass balances, the gas flow through the sample train was added to that metered at the PCS system outlet. During steady state operation, the gas flow through the sample train was metered with a test meter, and the water condensed in the train was measured and used as the primary measurement of the water content of the reactor make gas. Gas samples were taken in both stainless steel and glass bombs for GC analysis.

The gas sample train was designed to allow representative samples of particulates, tars, and condensed liquids to be taken. It was also necessary, especially in the case of trace element analysis, to trap all of the particulates, tars, and condensed liquids in one location to minimize sample contamination. For this purpose, a cold trap was installed in the sample train, which consisted of a vertical stainless steel cylinder, equipped with gas inlet and exit ports, and a drain-plug to drain the condensed liquids. The cylinder was loosely packed with stainless steel wool, which trapped the particulates and tars as the gas travelled through it. The entire trap was immersed in an ice bath. The liquid collected at the bottom of the cylinder was drained at the end of the run. When the gasifier reached steady-state, the cold trap was opened and the sample-train gas was diverted through it for one hour. At the end of the run, the contents of the trap were separated into solid, tar, and liquid fractions, and sent for analysis.

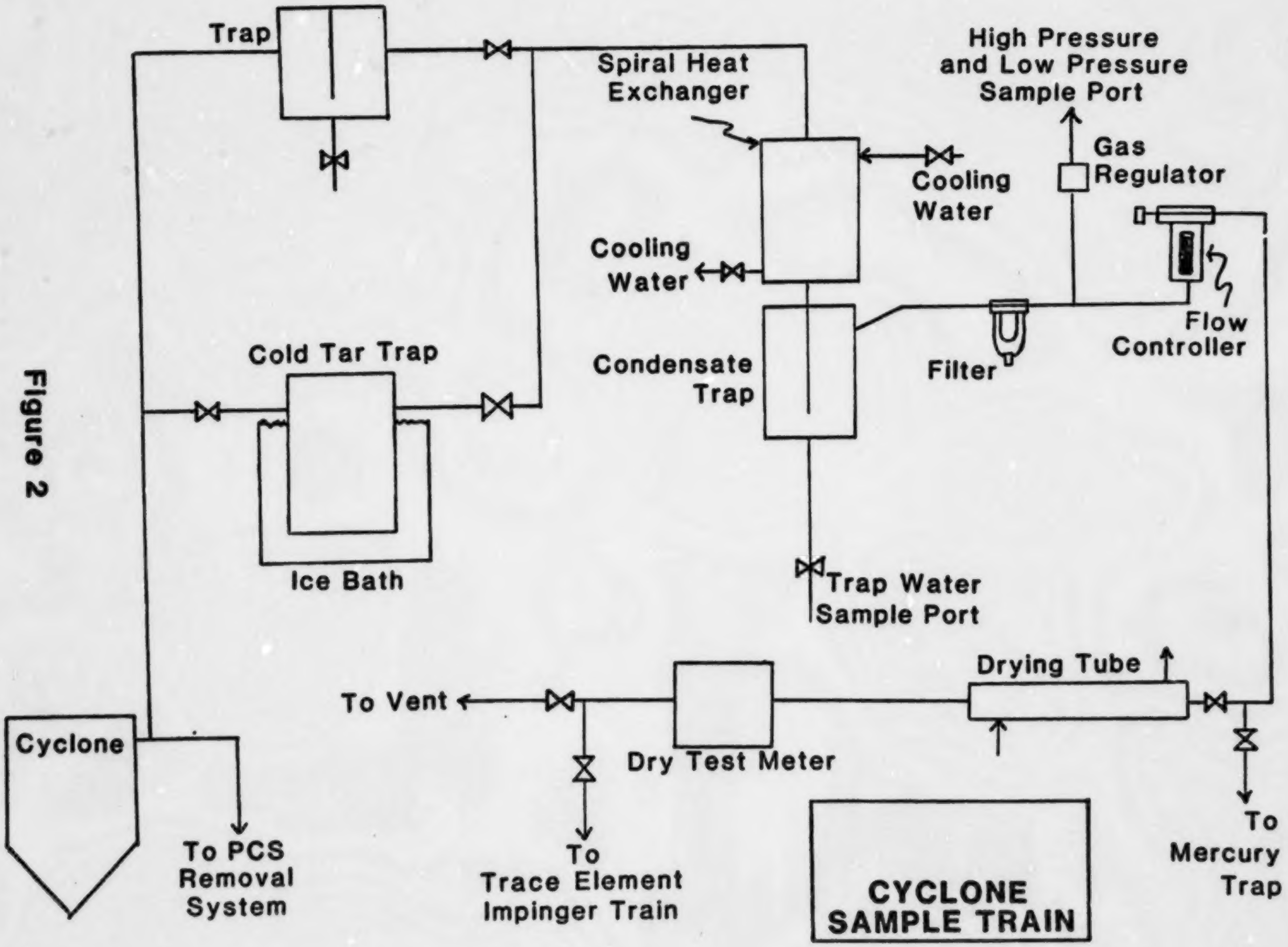

Trap
Spiral Heat Exchanger
High Pressure and Low Pressure Sample Port
Gas Regulator
Cooling Water
Cooling Water
Flow Controller
Cold Tar Trap
Condensate Trap
Filter
Ice Bath
Trap Water Sample Port
Drying Tube
To Vent
Cyclone
Dry Test Meter
To PCS Removal System
To Trace Element Impinger Train
CYCLONE SAMPLE TRAIN
To Mercury Trap

Figure 2

ANALYTICAL PRODEDURES

SOLIDS

Both proximate and ultimate analyses were performed on all solid input and output streams. The proximate analyses were performed using a Fisher Coal Analyzer Model 490. A Lindberg Combustion Furnace Model 123-SP was used to determine carbon and hydrogen for the ultimate analyses, and a Fisher Sulfur Analyzer Model 470 was used for sulfur analysis. Nitrogen was determined by the Kjeldahl-Gunning method, and oxygen was determined by difference. Certified coal standards were analyzed periodically to check the accuracy of all analyses.

LIQUIDS

The methods used for the analysis of the waste water, both the water from the PCS tank and from the sample train are listed below:

1. Ammonia - Acidimetric method 418D (Franson 1975). The sample pH was adjusted, it was distilled into boric acid, and then titrated with 0.1N H_2SO_4.
2. Cyanate - Pretreatment and heating was by method 413J (Franson 1975), distillation and titration was by method 418 (Franson 1975).
3. Carbon, TOC and TVC (Total organic carbon and total volatile carbon) - Samples were analyzed by a Dohrmann Envirotech Organic Carbon Analyzer. Samples were preserved by adjusting the pH to 2.0 with HCL. Thirty uL injections of the sample and KHP standards were used.
4. Chloride, Fluoride, Sulfate, Sulfite - Analysis was by a Dionex System 10 Ion Chromatograph. Identification was by retention time comparison with standards. Concentrations were determined by calibration curves (micro-moles versus peak height) of standards.
5. COD (Chemical oxygen demand) - Analysis was by the Hach COD System, a compact system in which the dichromate reflux takes place in a small sealed vial. A titration determined the reacted dichromate, and thus the COD.

6. Nitrogen - Samples were analyzed by method 421 (Franson 1975). The sample was digested to convert the organic nitrogen to ammonia (Kjeldahl), then distilled and titrated as in ammonia determination.

7. pH - Samples were determined by an Orion Microprocessor Ionalyzer 901. Calibration was with Fisher buffer solutions, and pH was determined with an Orion combination electrode.

8. Phenols - Analysis was by method 510c (Franson 1975). Phenols were reacted with 4-aninoantipyrine at pH 10 in the presence of potassium ferricyanide to form a colored antipyrine dye. The color was measured at 510 nm and plotted against standards.

9. Thiocyanate - Analysis was by method 413k (Franson 1975). The ferric ion was reacted with thiocyanate at acid pH to give an intense red color which could be read at 480 nm and plotted against standards.

In addition to the liquid analysis methods described above, the Research Triangle Institute carried out several analyses of PCS and Trap water, several analyses of tars collected from either the sample train cold trap or the PCS tank, and several samples of methanol from the AGRS. Analytical methods for the RTI analyses will be described with the results later in this report.

GASES

Gas Analysis Methods

Hydrogen, nitrogen, oxygen, carbon monoxide, carbon dioxide, methane, ethane, ethylene, and hydrogen sulfide (in relatively high concentrations) were analyzed on a Carle Series SX AGC-111H gas chromatograph in conjunction with a Perkin-Elmer Sigma 10 Chromatography Data System. The AGC-111H is a dual valve, dual column, dual detector unit. Gases were injected through the first valve, which could also be switched for a column backflush. A second valve is located between the two columns and switches to align them in series or bypass flow to the second column. The first column is 6′ x 1/8" 80% Poropak N and 20% Poropak Q. The second column is 7′ x 1/4" Molecular Sieve 13X. A third column, 8% OV101 Chromasorb WAWDMCS, is used as a reference column. Columns were maintained at 75°C throughout the analyses.

Detection of all the above mentioned gases except hydrogen was performed with a thermal conductivity (TC) detector with helium carrier gas. Hydrogen was separated from the other gases by permeation through a palladium-tube transfer system. A second TC detector, using nitrogen carrier gas, detected H_2 at concentrations from 0.03% to 100%. The currents in both detectors were set at 20 mA. The Perkin-Elmer Sigma 10 Chromatography Data System performed automated valve switching and peak area integration. An example of a chromatogram from the Carle-Sigma 10 for the 15:30 sample train gas sample of June 10, 1981, Run GO-79, is shown in Figure 3.

Hydrogen sulfide, carbonyl sulfide, methyl mercaptan, ethyl mercaptan, carbon disulfide, and thiophene were analyzed on a Varian gas chromatograph. A gas sampling valve was added for sample injection. Sample components were separated on a 6′ x 1/8" teflon 1.5% x E-60, 1% H_3PO_4 Carbopak B column which was temperature programmed. The column was held at 25°C for 3 minutes, heated to 130°C at 15°C per minute, and held at 130°C for 6 minutes.

Detection of sulfur gases in the high hydrocarbon coal matrix was accomplished using a Varian dual-flame flame photometric detector. The detector was heated to 180°C and used helium as carrier gas and hydrogen and air as flame gases. An example of a chromatogram of the PCS sample at 11:40 on June 10, 1981, GO-79 is shown in Figure 4.

Ethane, ethylene, all C3 and C4 hydrocarbons, and methanol were analyzed on a Tracor 550 gas chromatograph. A gas sampling valve and valve oven were added for sample injection. The sample components were separated on an 8′ x 1/8" stainless steel Poropak Q column in series with an 10" x 1/8" stainless steel 20% Carbowax 20M TPA column. The columns were temperature programmed from 50°C to 200°C at 8°C per minute. The gases were detected by a flame ionization detector heated to 250°C. Helium was used as the carrier gas. A sample chromatogram of the AGRS feed gas from GO-79 is shown in Figure 5.

Benzene and toluene were analyzed on a Tracor 550 gas chromatograph with a heated gas sampling valve for injection. A 7′ x 1/8" stainless steel 35% BC 150 Chromasorb PAW, DMCS column separated benzene and toluene. The column was temperature programmed from 120°C to 200°C at 8°C per minute. Components were detected by a flame ionization detector heated to 250°C. Helium was used as the carrier gas.

For all the gas chromatographic analyses, the Perkin-Elmer Sigma 10 Chromatography Data Station received all detector outputs and integrated to calculate peak areas. The peak areas were converted to micromoles and mole % by external standard calibration curves in a series of steps using a Hewlett Packard 97 programmable calculator and the SAS statistical program. Final compilation and storage of data was accomplished by means of the GASS computer program described below.

In addition to the gas analyses described above, the Research Triangle Institute, Research Triangle Park, NC, performed complete gas analyses for several runs.

GASS Computer Program

GASS is an interactive data reduction system designed to process, log, and retrieve gas chromatography data, and to generate reports of gas analysis results. GASS routines are written in Applied Information Systems (AIS) PL/I.

Figure 3

CHROMATOGRAM FROM THE CARLE GC

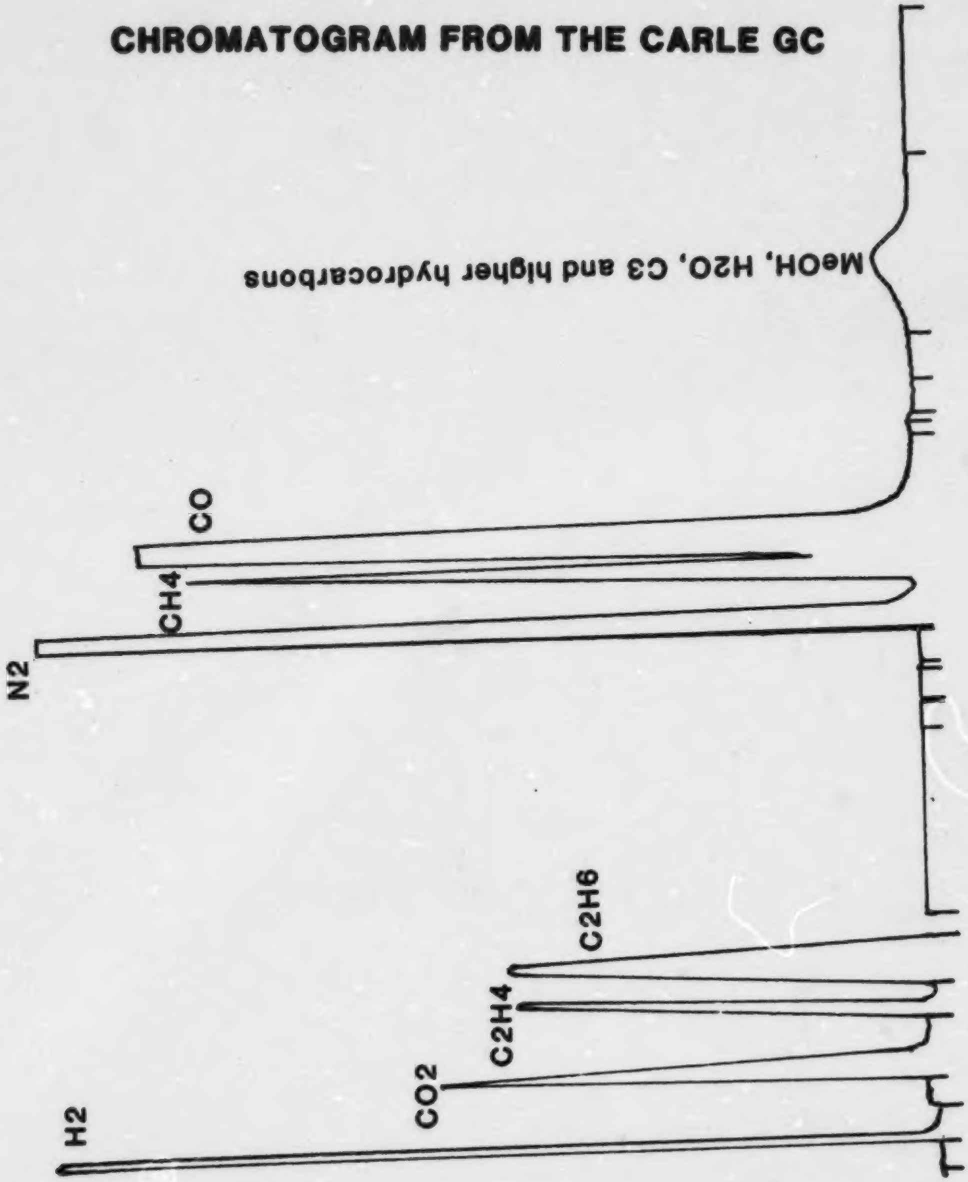


Figure 4
CHROMATOGRAM FOR
SULFUR GASES FROM VARIAN GC

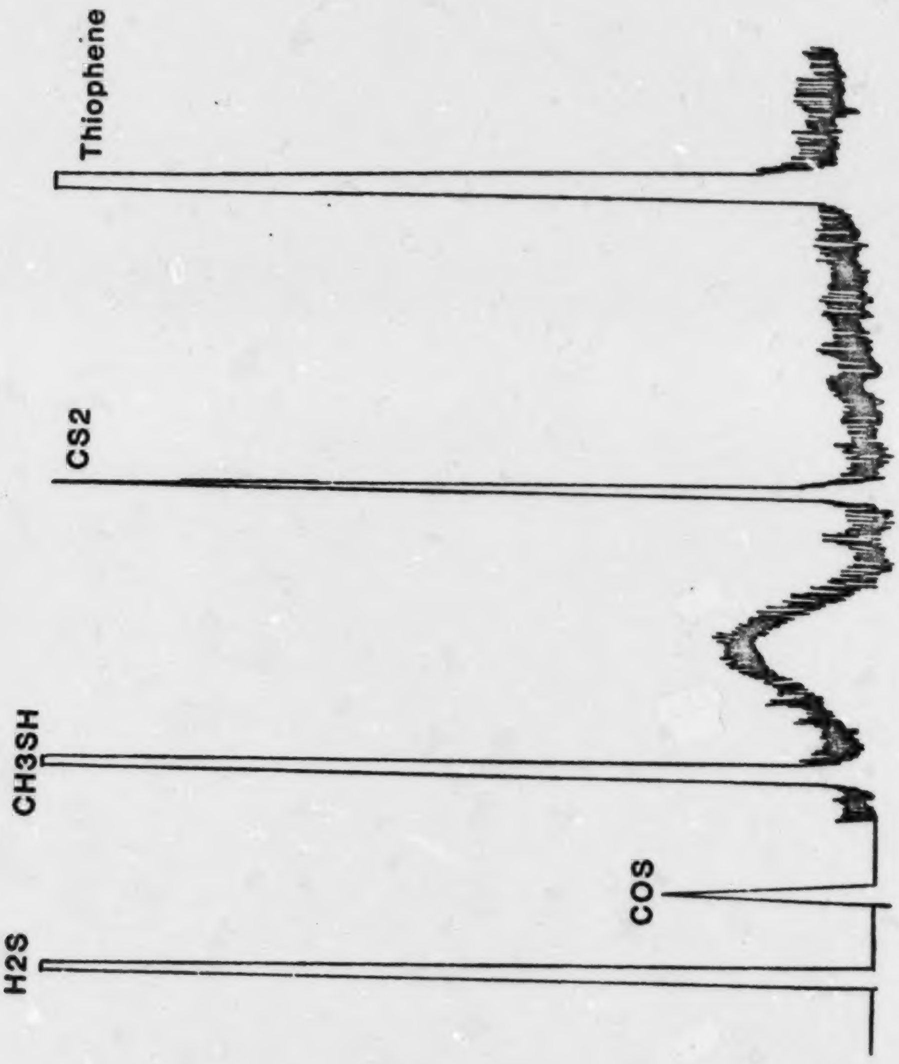
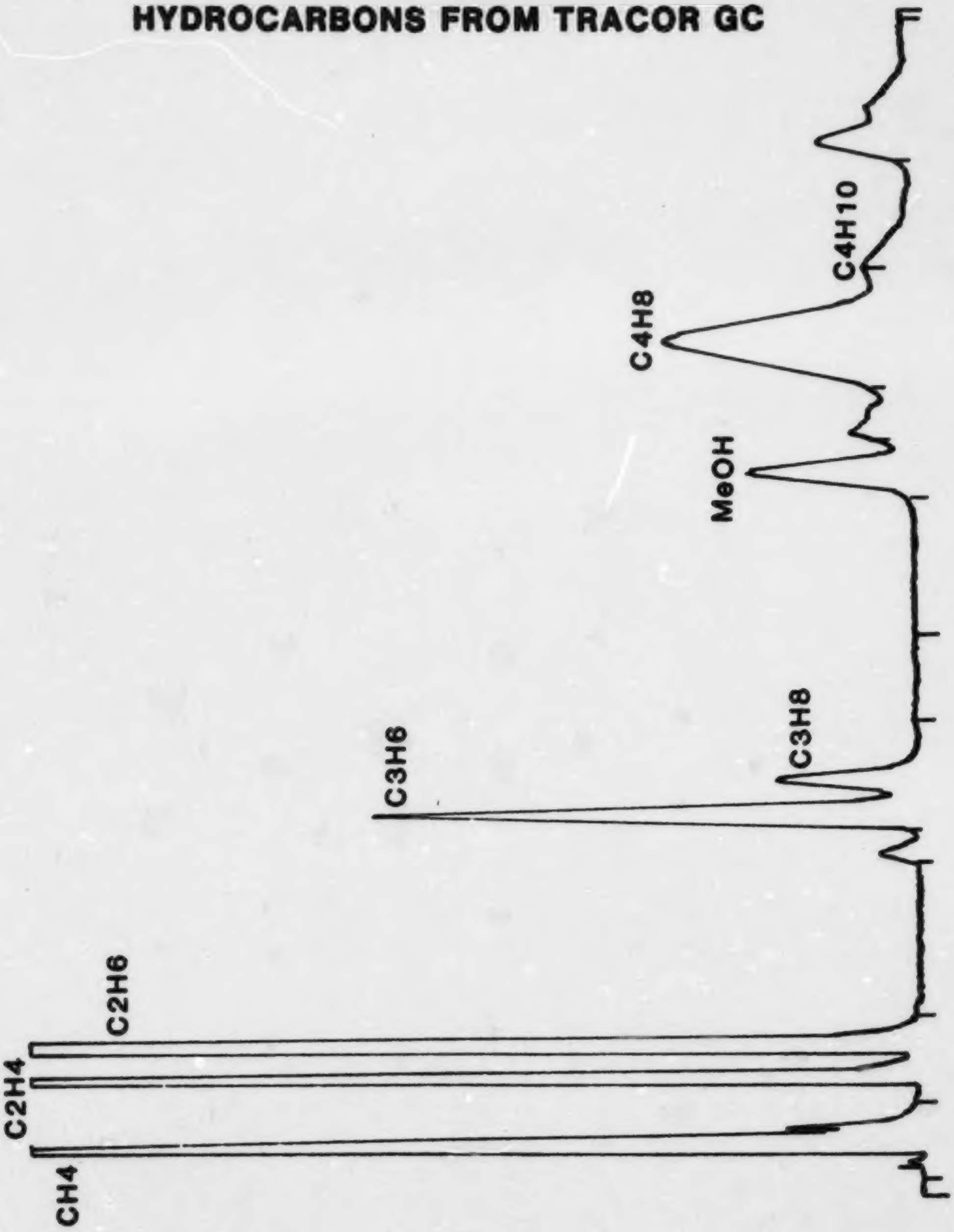


Figure 5

CHROMATOGRAM FOR HYDROCARBONS FROM TRACOR GC



An example of the output of the GASS program is given in Table 2 for the analysis of the 15:30 sample train gas sample from GO-79. Two replicate analyses are shown in the table. Also shown are the calibration curves used for the calculation of composition from peak areas. The percent recovery is calculated by totaling the micromoles calculated from the calibration curves and the peak areas, and dividing by the total micromoles injected from the gas sample loop. Since not all compounds present in the sample were included in the analysis, the percent recovery calculated for this sample is less than 100%.

TRACE METAL SAMPLING AND ANALYSIS

Feed coal, spent char, and cyclone fine samples were routinely collected and analyzed for arsenic, lead, and mercury. In addition, a small stream from the gas leaving the cyclone was diverted through the cold trap and/or a series of impingers and/or a series of gold amalgamation columns, all of which generated samples which were then analyzed for trace element content. A schematic diagram of the sample train used for trace metals is shown in Figure 6.

Solids were prepared for analysis by digesting one-gram samples in a Parr bomb under 30 atmospheres of O_2, with enough concentrated HNO_3 to have 0.5% HNO_3 in the final dilution. After cooling, the liquid in the bomb was rinsed into a 100 ml volumetric flask and diluted to volume.

Following a run, the cold trap described earlier was opened and the packing was removed and its weight recorded. The packing was then soaked in about 1500 ml of HPLC-grade methylene chloride, which dissolved the tars and removed the particulates from the packing. The extract was then filtered and the residual solids were dried and weighed. The weight of tar was estimated from the net weight of the packing and the weight of recovered solids.

The methylene chloride solution containing the tar was evaporated down until all the solvent had been driven off, and the tar was then digested following the same procedure used for the solids. The tar trap water was digested by heating it with enough added HNO_3 to break down the organic constituents, which would otherwise cause interference in the spectrometric analysis.

An unsuccessful attempt to capture arsenic and lead from the make gas over and above the amounts recovered in the cold trap was made. A gas stream was bubbled through a set of three modified Greenburg-Smith impingers, each containing a 10% HNO_3 solution. All three impingers were placed in an ice bath, to enhance gas solubility. The solution was later changed to 0.01M EDTA in 10% HNO_3, with a view toward chelation of the trace metals. The system, which in early tests appeared to show promising results, failed to yield measurable amounts of either trace element.

TABLE 2
NCSU COAL GASIFICATION PROJECT
GAS CHROMATOGRAPHY - GAS BOMB ANALYSIS   6/10/81

```
RUN NUMBER:  GO-79                         RUN DATE:  6/10/81
BOMB NUMBER:  28                           SAMPLE LOCATION: SAMPLE TRAIN
SAMPLE TIME:  15:30                        ANALYST:  K. STEINSBERGER
DETECTOR:  TCD                             INSTRUMENT:  CARLE
T = 348 K                                  P =  5.00 PSIG
LOOP SIZE =  1.00 ML                       DILUTION FACTOR =  1.00

                        CALIBRATION CURVES USED:
  H2      6/15/81       .07< [A] <  7.19      r =  .998
  MIC-MOLES =  0.0000E+00*[A]**3 +  0.0000E+00*[A]**2 +
               4.5396E+00*[A]** 1.0000E+00 + -4.0138E-01

  CO2     6/15/81      2.00< [A] < 25.00      r =  .998
  MIC-MOLES =  0.0000E+00*[A]**3 +  0.0000E+00*[A]**2 +
               3.4811E-01*[A]** 1.0000E+00 +  6.7094E-01

  CH4     6/22/81      3.00< [A] < 25.00      r =  .998
  MIC-MOLES =  0.0000E+00*[A]**3 +  0.0000E+00*[A]**2 +
               6.8498E-01*[A]** 1.0000E+00 + -1.8341E-02

  C2H4    6/19/81       .50< [A] <  3.00      r =  .998
  MIC-MOLES =  0.0000E+00*[A]**3 +  0.0000E+00*[A]**2 +
               3.4883E-01*[A]** 1.0000E+00 +  1.7161E-03

  C2H6    6/19/81       .50< [A] <  3.50      r =  .998
  MIC-MOLES =  0.0000E+00*[A]**3 +  0.0000E+00*[A]**2 +
               3.2301E-01*[A]** 1.0000E+00 +  9.7865E-04

  N2      6/15/81      2.00< [A] < 70.00      r =  .998
  MIC-MOLES =  0.0000E+00*[A]**3 +  0.0000E+00*[A]**2 +
               4.4747E-01*[A]** 1.0000E+00 + -5.3289E-01

  CO      6/15/81      1.29< [A] < 60.00      r =  .998
  MIC-MOLES =  0.0000E+00*[A]**3 +  0.0000E+00*[A]**2 +
               4.3860E-01*[A]** 1.0000E+00 +  5.5563E-02

  H2S     7/2/81        .69< [A] <  2.00      r =  .998
  MIC-MOLES =  0.0000E+00*[A]**3 +  0.0000E+00*[A]**2 +
               4.6802E-01*[A]** 1.0000E+00 +  1.7669E-02
```

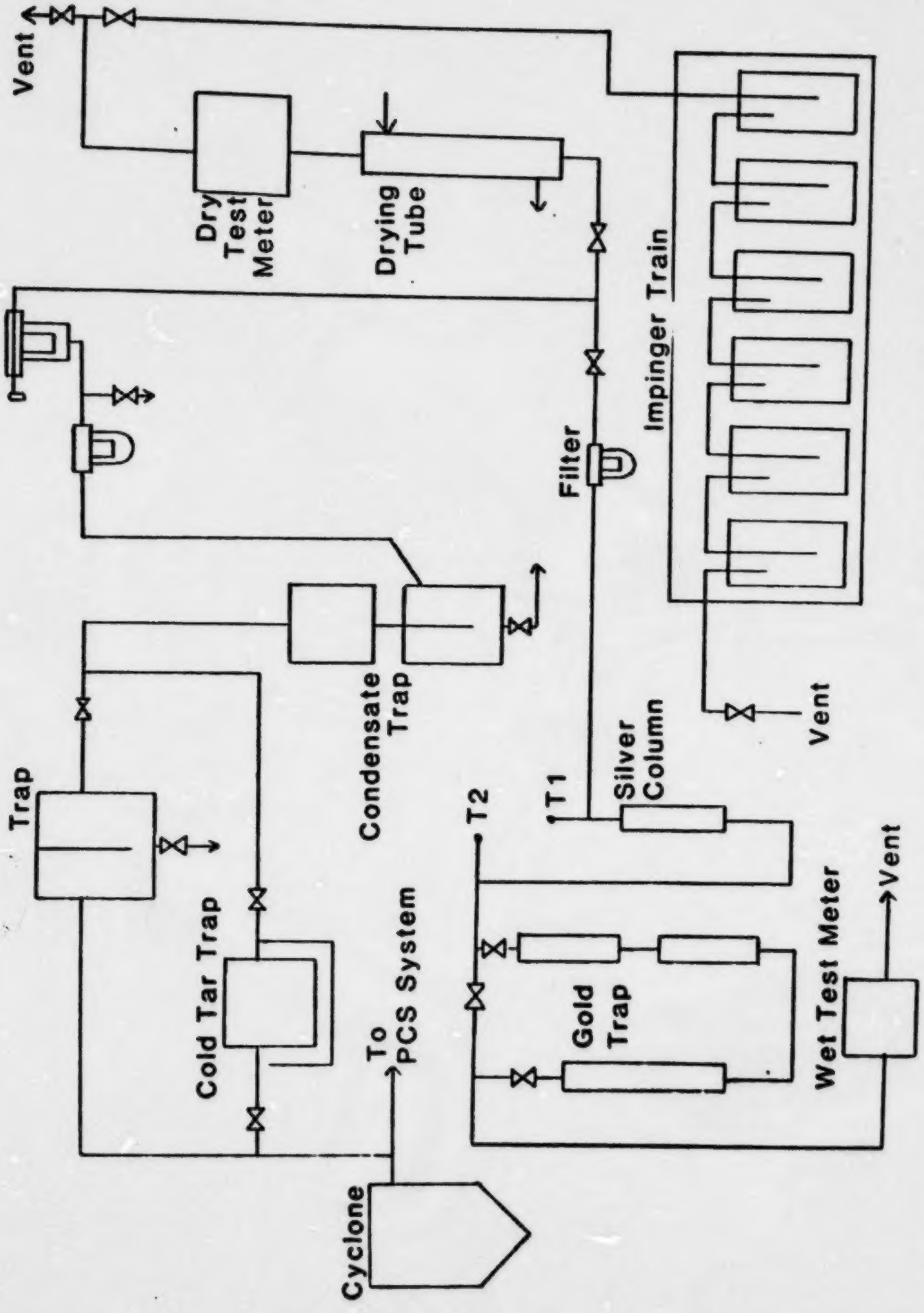
TABLE 2 CONTINUED
GO-79 6/10/81
BOMB 28 GAS COMPOSITION
SAMPLE TRAIN 15:30

COMPOUND	AREA	MICROGRAM MOLES	MOLE PERCENT
SAMPLE 1			
H2	3.1926	14.0917	31.8759
CO2	25.4758	9.5393	21.5782
C2H4	.5501	.1936	.4380
C2H6	.6490	.2106	.4764
H2S	.0032	.0192	.0434
O2	.0000	.0000	.0000
N2	22.1350	9.3718	21.1994
CH4	4.8203	3.2835	7.4274
CO	16.9688	7.4981	16.9609
MICRO-MOLES INJECTED	46.9341		
PERCENT RECOVERY	94.19%		
SAMPLE 2			
H2	3.2035	14.1412	31.9899
CO2	25.3824	9.5068	21.5060
C2H4	.5496	.1934	.4375
C2H6	.6477	.2102	.4755
H2S	.0041	.0195	.0443
O2	.0000	.0000	.0000
N2	22.1177	9.3641	21.1832
CH4	4.8150	3.2798	7.4195
CO	16.9503	7.4900	16.9437
MICRO-MOLES INJECTED	46.9341		
PERCENT RECOVERY	94.18%		

STATISTICAL MOLE PERCENT ANALYSIS BOMB 28
SAMPLE TRAIN 15:30 6/10/81

COMPOUND	MEAN	DEVIATION	+LIMIT	-LIMIT
H2	31.9329	.0805	32.6570	31.2088
CO2	21.5421	.0510	22.0006	21.0836
C2H4	.4378	.0003	.4406	.4349
C2H6	.4760	.0006	.4818	.4701
H2S	.0438	.0006	.0492	.0384
O2	.0000	.0000	.0000	.0000
N2	21.1913	.0114	21.2939	21.0887
CH4	7.4235	.0055	7.4736	7.3733
CO	16.9523	.0122	17.0620	16.8426

Figure 6


Vent
Dry Test Meter
Drying Tube
Impinger Train
Filter
Vent
Condensate Trap
Trap
Silver Column
T1
T2
Cold Tar Trap
To PCS System
Gold Trap
Wet Test Meter
Vent
Cyclone

TRACE ELEMENT SAMPLE SYSTEM

Mercury in the gas stream was captured using a gold packing, with which it formed an amalgam. The sampling system consisted of a filter for particulate removal, a silver catalytic oxidizer, three gold amalgamation columns in series, and a wet test meter for gas flow rate measurements. The oxidizer was maintained at a temperature of about 320°C to convert any alkyl mercury to elemental mercury, since the former does not amalgamate with the gold. The high temperature also prevents mercury from forming an amalgam with the silver.

Following a run, the gold packings were removed and each of the traps was heated in a tubular furnace at about 600°C under a small nitrogen flow, into which the mercury desorbed. The gas stream was bubbled through a solution containing acidified $KMnO_4$. The solutions were then stored for subsequent Hg cold vapor analysis.

All trace element analyses were carried out using a Perkin-Elmer Model 603 Atomic Absorption Spectrophotometer. An HGA-2200 graphite furnace was used for the analyses of arsenic and lead, while mercury was determined by a cold vapor method. Ramp heating was used for the drying and charring steps, and normal, temperature controlled, or time controlled heating was used during atomization. Deuterium background correction was used for arsenic and lead analyses. Electrodeless Discharge Lamps were employed in all cases.

For arsenic determination, the wavelength and slit width were set at 197.2 and 0.7 nm respectively. Fifty ul samples were introduced into the furnace and were then dried at 125° C for 50 seconds, charred at 1000° C for 30 seconds, and atomized at 2700° C for 8 seconds. The ramp time for the drying and charring steps were 10 seconds each. A pyrolitically coated furnace tube was used for arsenic to provide greater durabiliy at the higher atomization temperature. Nickel complexation was also used to allow high temperature charring.

For lead determination, the wavelenth and slit width were set at 217.0 and 0.7 nm respectively. Twenty ul samples were dried at 125° C for 20 seconds, charred at 600° C for 45 seconds, and atomized at 2300° C for 8 seconds. The ramp time for the drying and charring steps were 10 seconds each. The method of standard additions was used for both arsenic and lead analyses.

Direct calibration methods were employed for the analysis of mercury. The wavelength and slit width settings for mercury were 254 nm and 0.7 nm respectively.

Methods used currently for arsenic analysis are satisfactory, both for ease of application and reliability. The principal problem associated with this element is the ineffectiveness of the impinger solutions at trapping it from the gas stream. Reproducibility of lead concentration measurements has been less than satisfactory, although considerable improvement has been made recently by diluting all samples to fall within the linear range of the instrument calibration, and by adding dibasic ammonium phosphate to the injected sample, thereby binding the lead and enabling higher charring temperatures. The cold-vapor technique used for mercury is satisfactory; the principal difficulty associated with this element is its volatility, which makes it essential to analyze samples close to the times at which they were taken.

MASS BALANCES AND QUALITY ASSURANCE

Mass balances for both the gasifier and the acid gas removal system are given in Appendices A and E. In general, the mass balance results are excellent, and indicate that there are no gross errors in either chemical analyses or mass flow measurements. Frequent calibration checks were necessary to achieve the mass balance results shown.

The mass balance program used for the results shown in the appendices used average values for all flow rates, pressures, temperatures, and stream compositions. These averages were computed from the data stored by the data acquisition system. In order to assure that the system was operating at a good steady state over the period of time used for the averaging program, selected data from the file were plotted versus time, and an appropriate time span was selected for the steady state. Examples of plots of some of the more sensitive process variables are shown in Figures 7 through 15 for run GO-79. Five different events are marked on the time axis of these graphs. The first of these, number 1, indicates the time at which a set of make gas samples was taken after the gasifier had been operating at steady state for approximately two hours. These early samples were taken to make sure of a good gasifier run in case of system failure before the AGRS reached steady state.

At approximately 13:00, event marker 2, the sour gas compressor was inadvertently turned off. The resulting upset in operation can be followed through the system. A good recovery was made from this upset, and full sets of gasifier and AGRS samples were taken at event markers 3 and 4. The system was shut down at 5. The duplicate sets of samples assure that good samples and analyses were achieved.

In addition to the quality assurance efforts mentioned above, all gas, solid, and liquid analyses were duplicated by carrying out at least two analyses for each sample.

GASIFIER BED TEMPERATURE AT 10 INCHES ABOVE BOTTOM

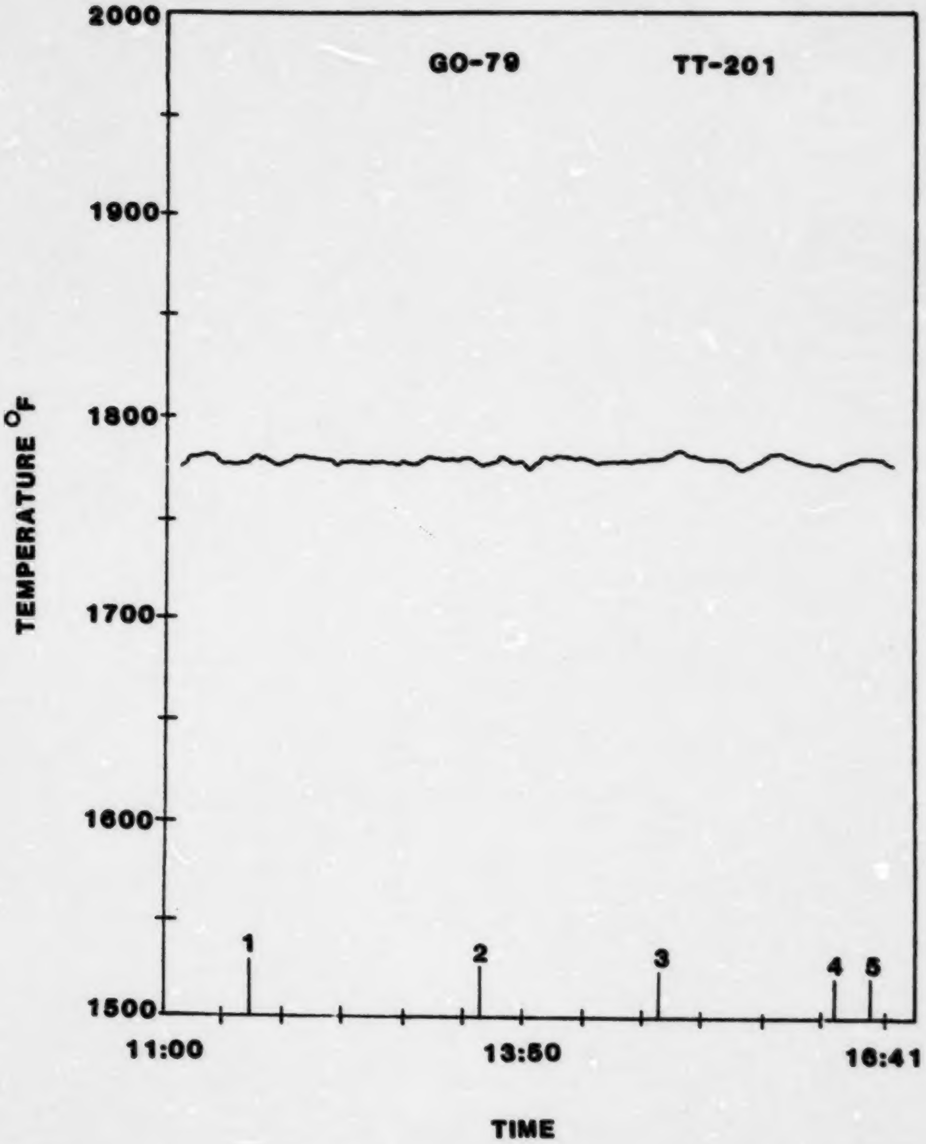


Figure 7

REACTOR MAKE GAS FLOW RATE

GO-79 FT-293

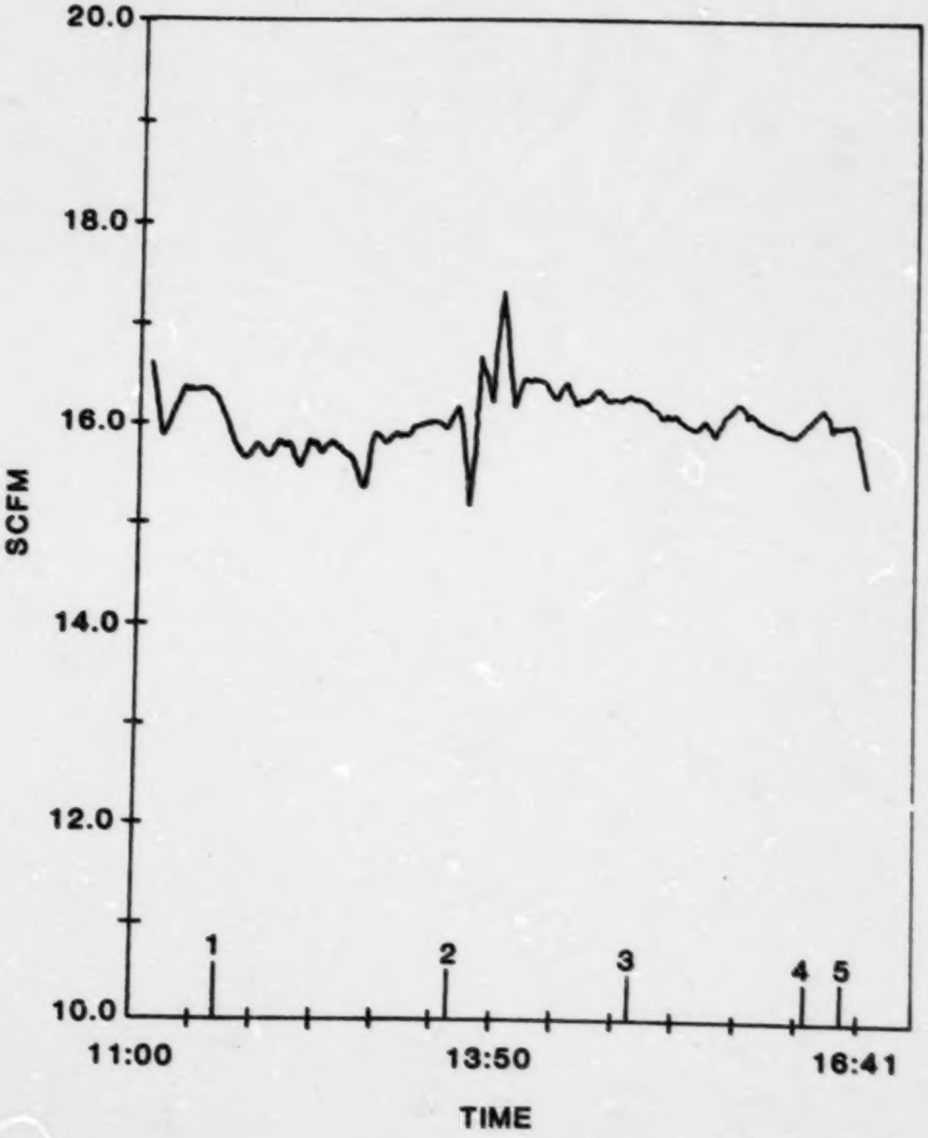


Figure 8

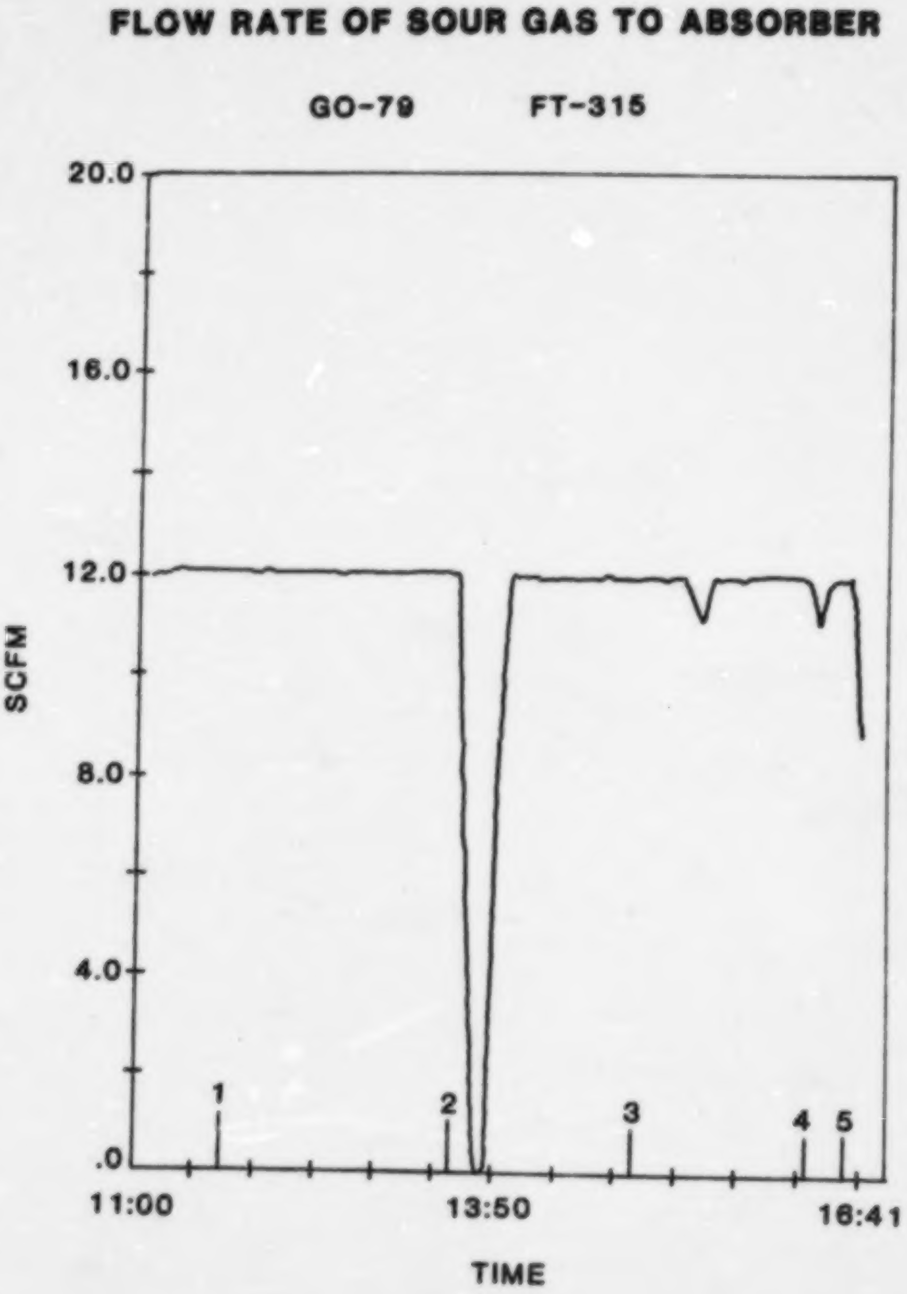
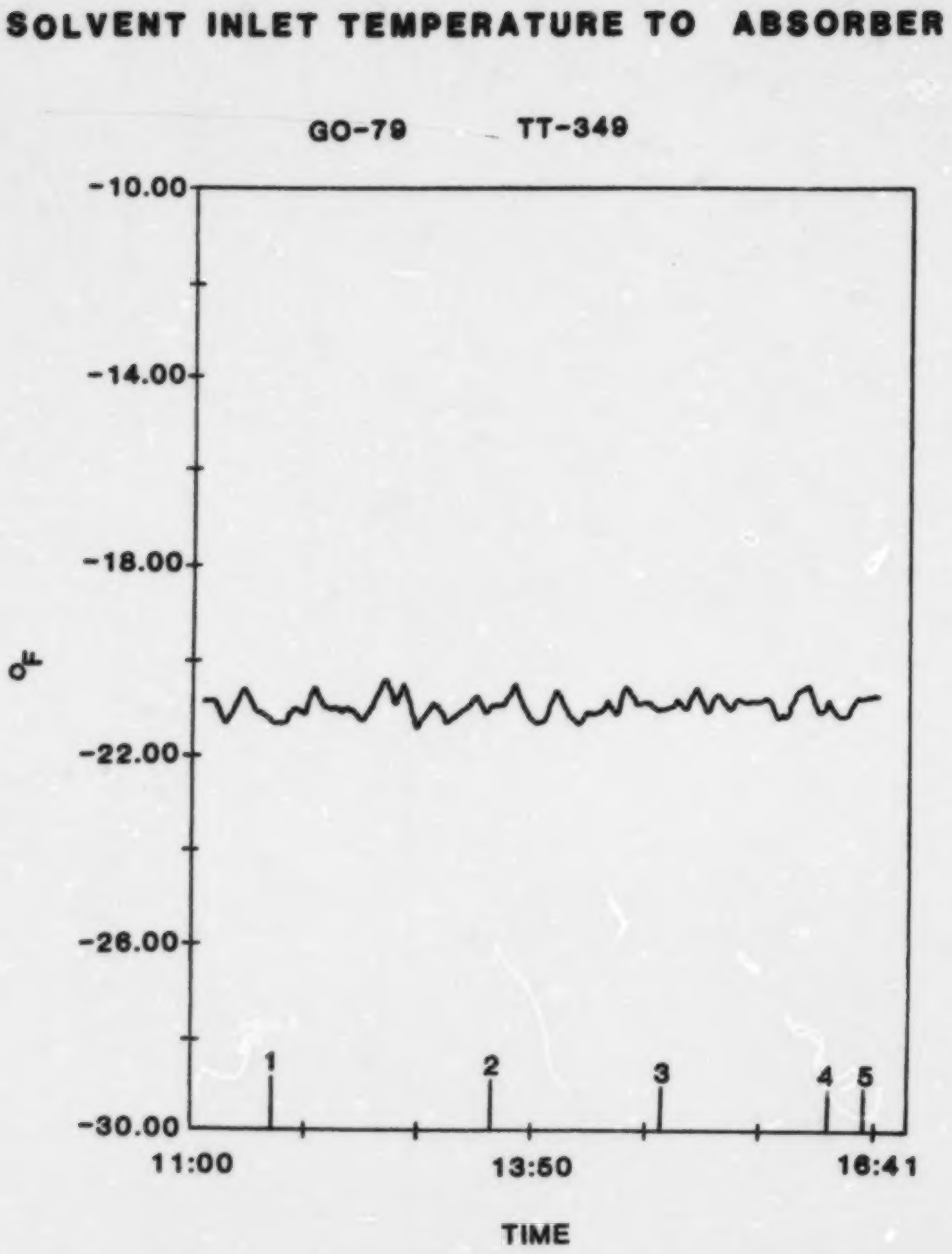

FLOW RATE OF SOUR GAS TO ABSORBER
GO-79
FT-315
20.0
16.0
12.0
8.0
4.0
.0
SCFM
1
2
3
4
5
11:00
13:50
16:41
TIME

Figure 9



SOLVENT INLET TEMPERATURE TO ABSORBER

Figure 10

Figure 11

ABSORBER PRESSURE

GO-79 PT-345

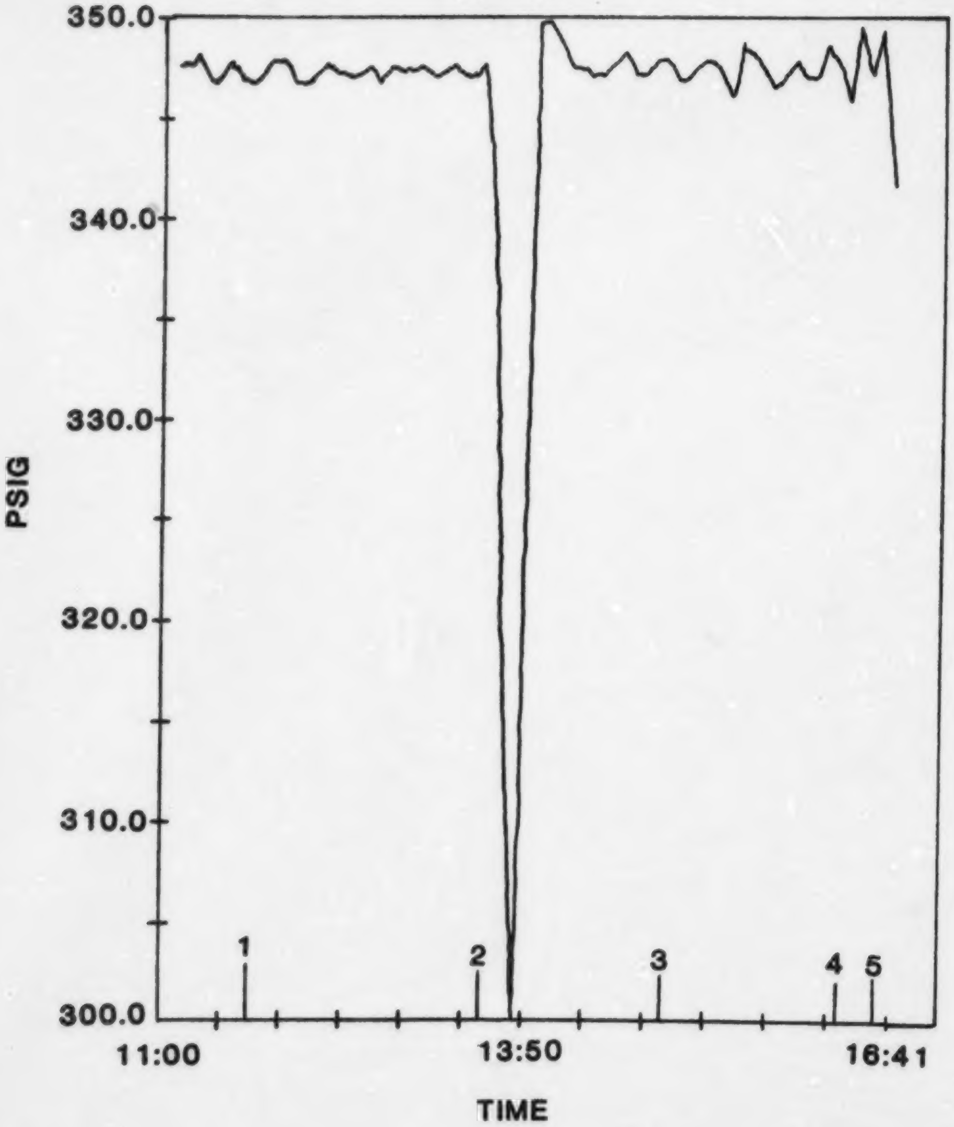
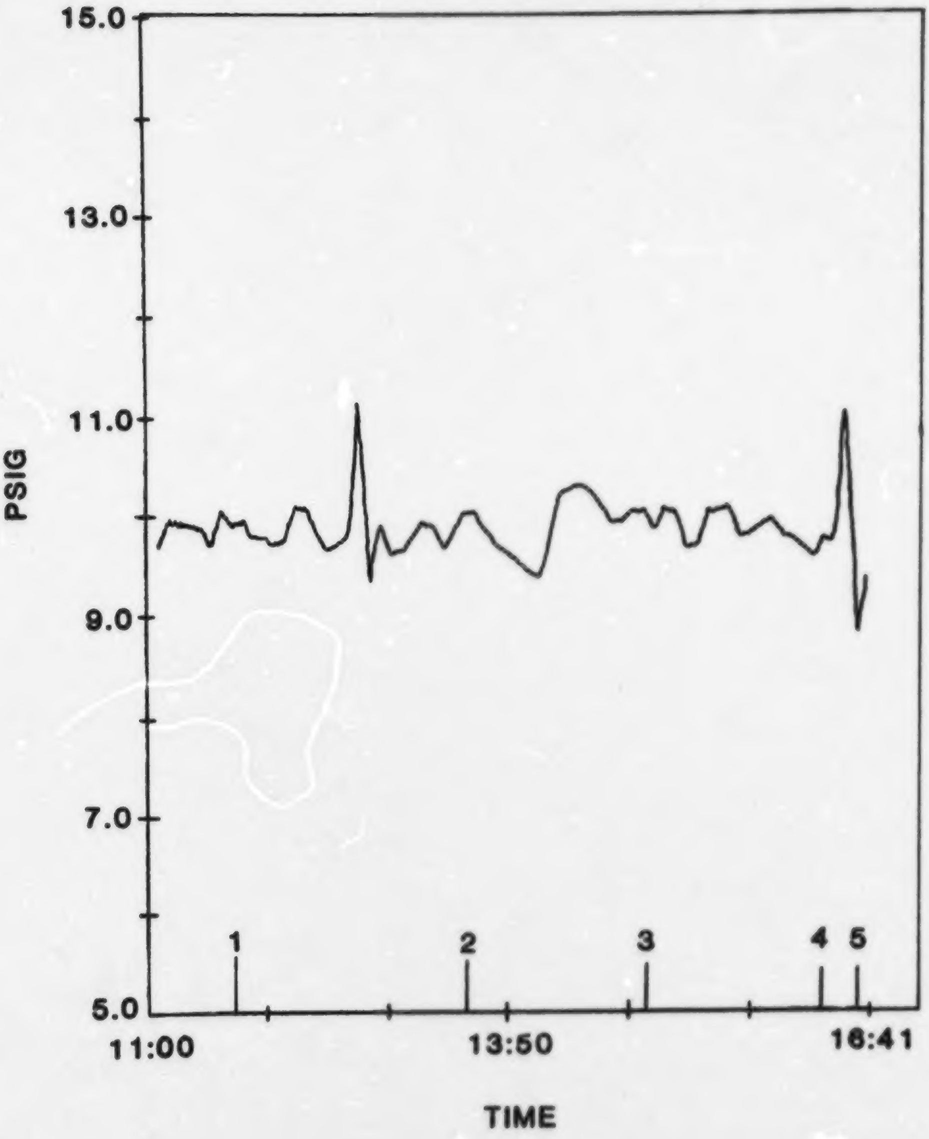


Figure 12

STRIPPER PRESSURE

GO-79 PT-370



SWEET GAS FLOW RATE FROM ABSORBER

GO-79 FT-345

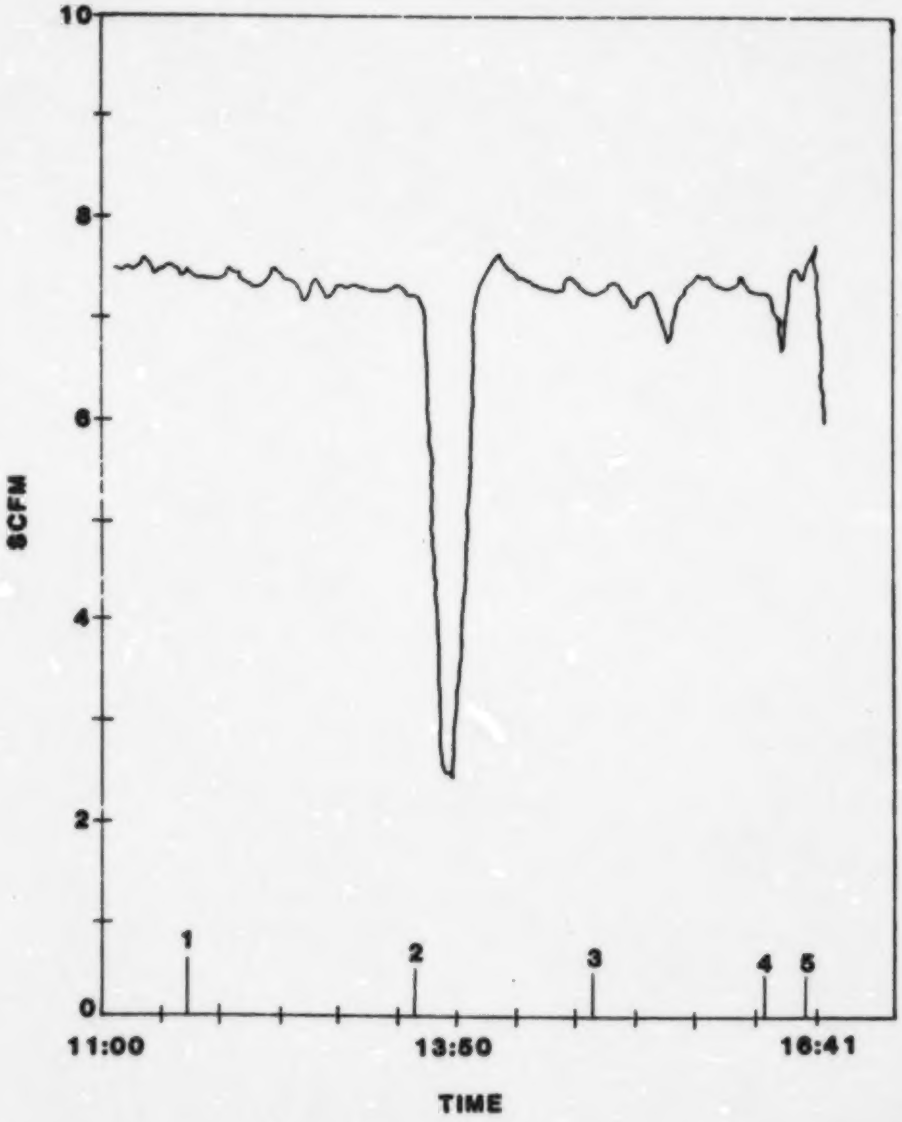


Figure 13

Figure 14

ACID GAS FLOW FROM STRIPPER

GO-79 FT-371

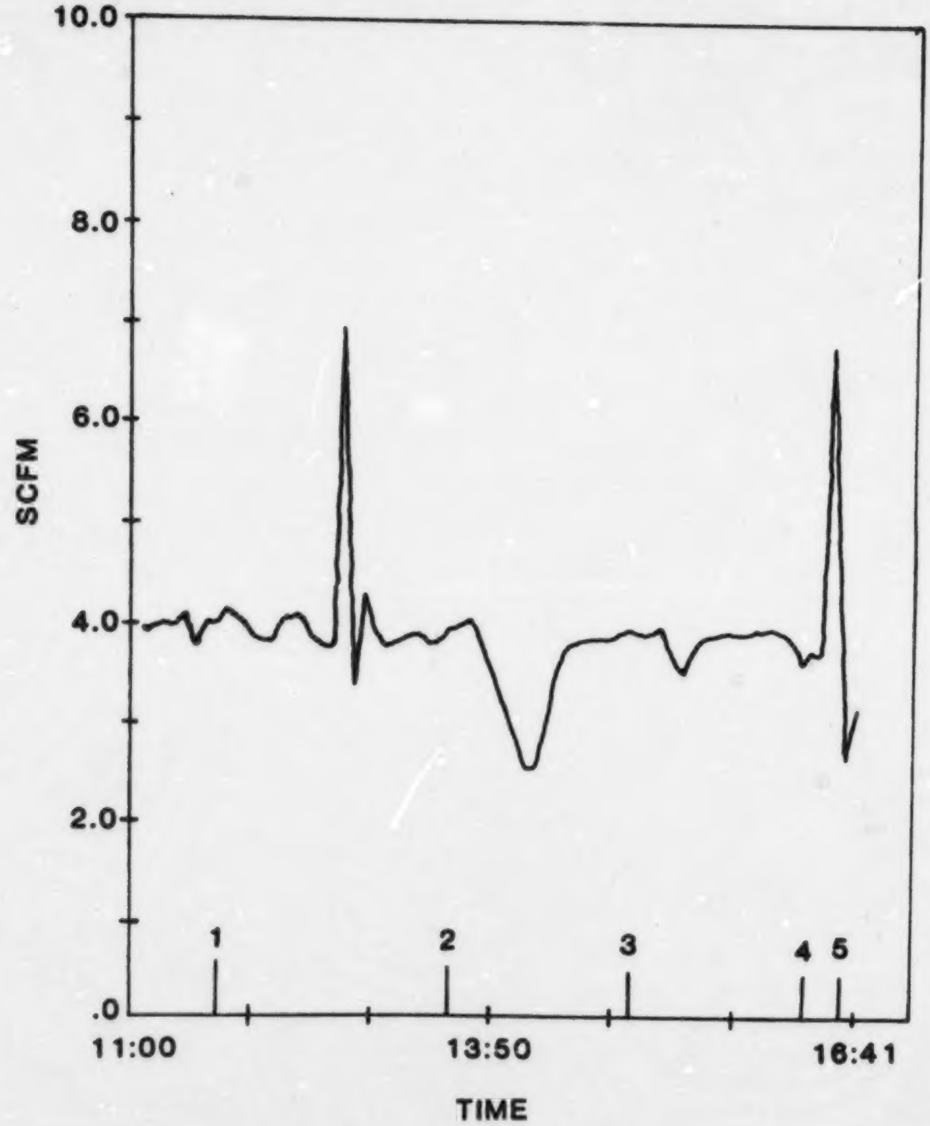
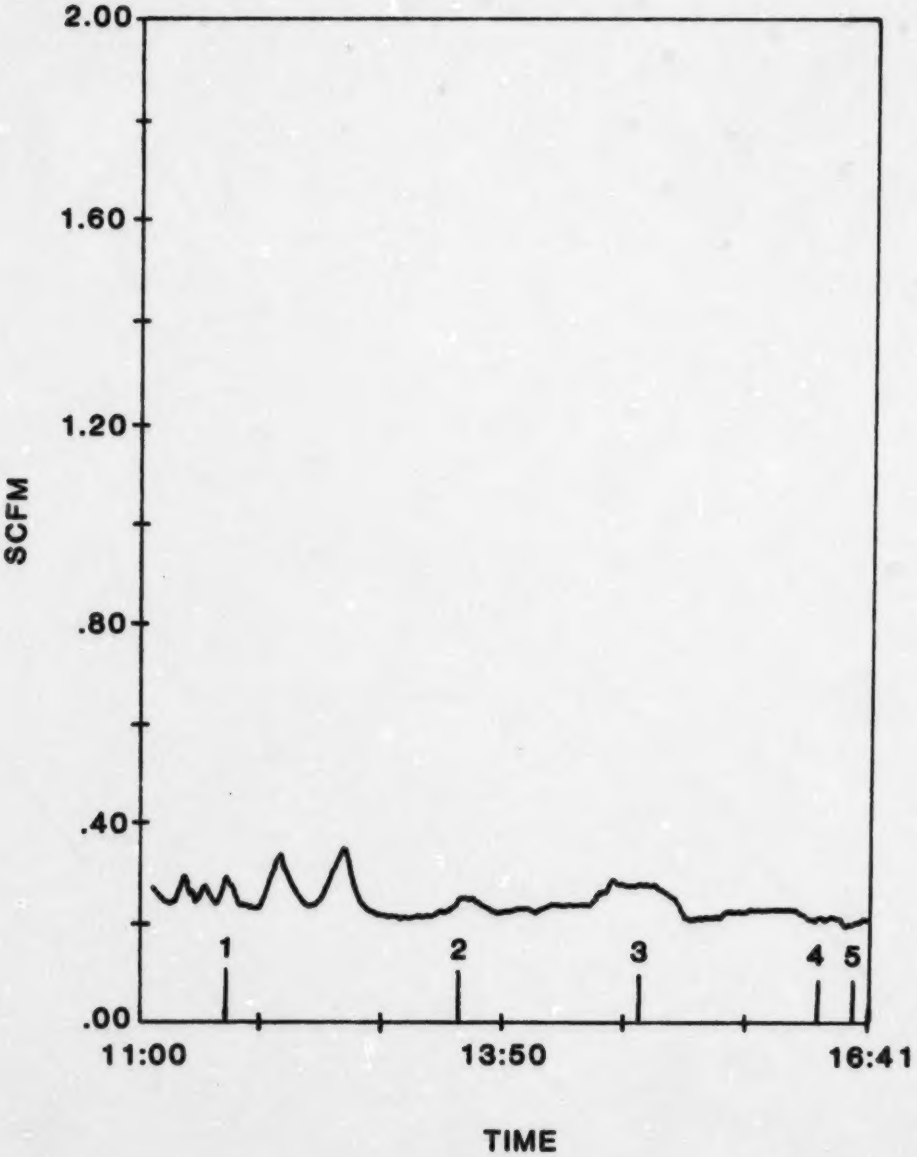


Figure 15
GAS FLOW RATE FROM FLASH TANK

GO-79 FT-358



EMISSIONS FROM THE GASIFIER-PCS SYSTEM

This section will review the results obtained for process stream analysis and for emissions from the gasifier-PCS system.

GAS STREAMS

Major Gases

Average values for all runs are reported in the tables of Appendices A through D. The effects of operating parameters on the production of the major gases will be discussed in the section on gasifier operation.

Sulfur Gases

Complete sulfur gas analyses for all runs are given in the tables in Appendices A through D. Sulfur gas emission rates, calculated as milligrams emitted per kilogram of coal fed, are plotted versus the average bed temperature in Figures 16 and 17. Despite scatter in the plots, it appears that the H_2S and COS emission rates show a slight increase with increasing temperature. The emission rates of the sulfur species in Figure 17 show no apparent dependence on temperature.

The coal char used in the work reported on in Volume II (Ferrell et al., 1981), had a volatile matter content less than 2%, and very likely most of the sulfur was present in an inorganic form. For this case it was postulated that during steam-oxygen gasification the gas-solid reactions formed mainly hydrogen sulfide. Gas phase reactions then tended to bring the compounds CO_2, H_2O, H_2, H_2S, and COS to an equilibrium mixture.

The two gas phase reactions of most importance involving H_2S and COS are:

$$COS + H_2O = H_2S + CO_2 \quad (1)$$

$$COS + H_2 = H_2S + CO \quad (2)$$

Figure 16

SULFUR GAS EMISSIONS

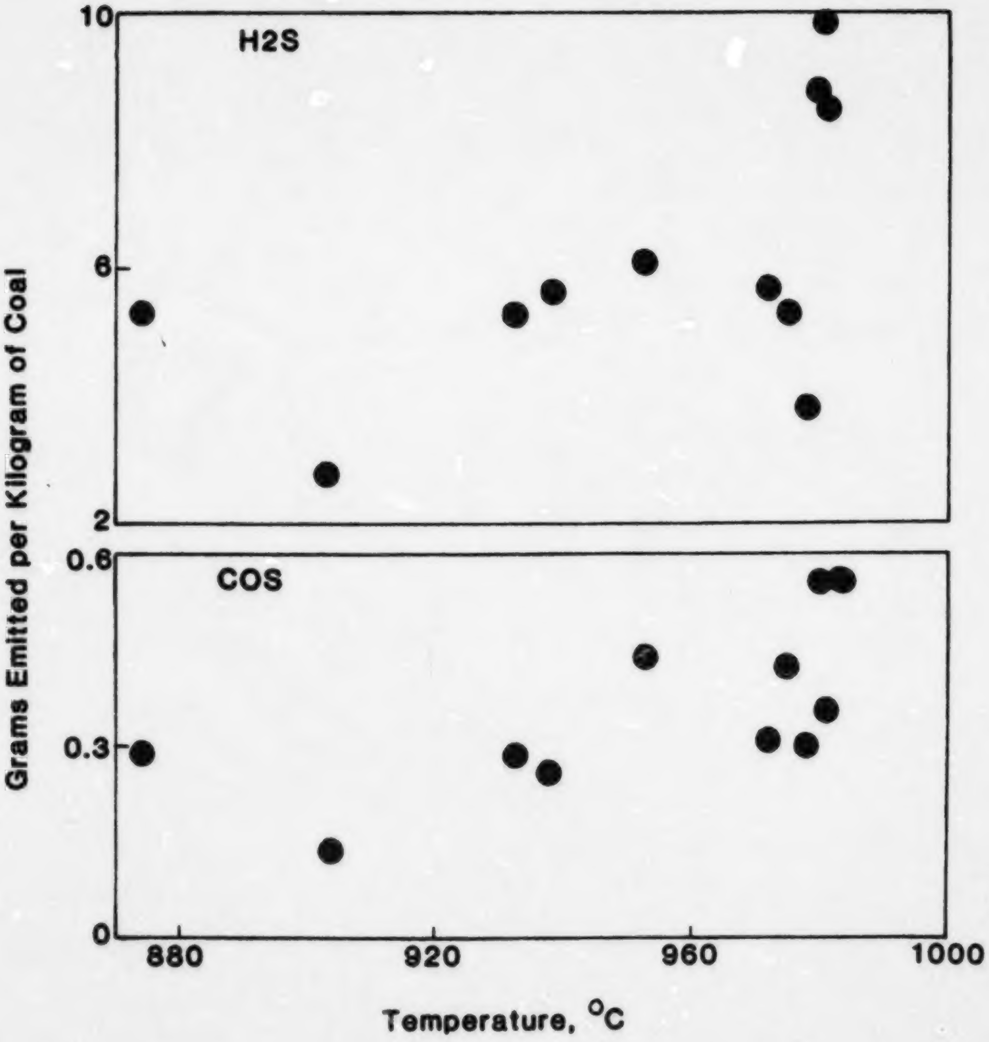
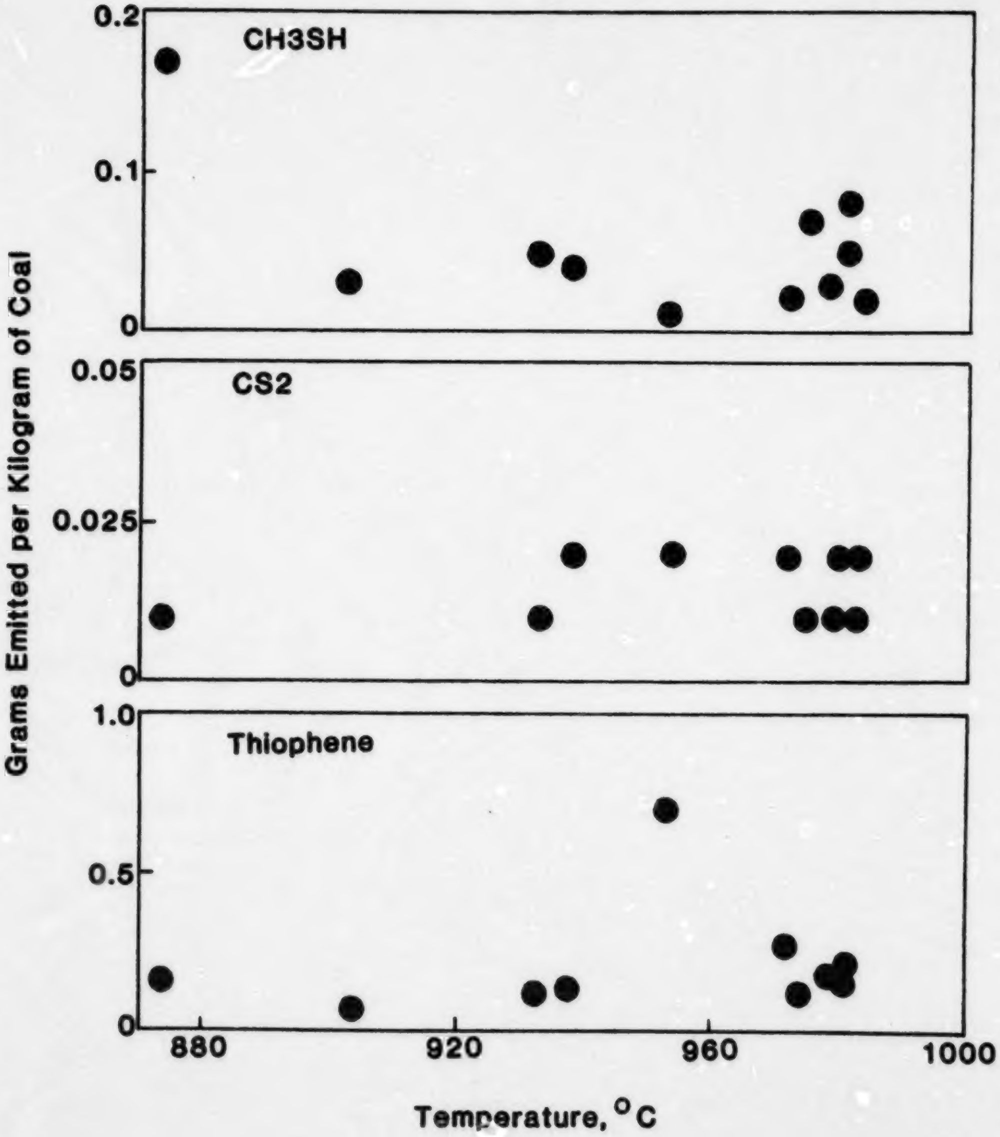


Figure 17

SULFUR GAS EMISSIONS



The equilibrium constants for these two reactions are defined as follows:

$$K_1 = [H_2S][CO_2]/[COS][H_2O] \quad (3)$$

$$K_2 = [H_2S][CO]/[COS][H_2] \quad (4)$$

where the brackets indicate any convenient concentration units. Ideal gas behavior is assumed.

Table 3 shows a compilation of all results obtained to date, and includes both char and New Mexico coal data. Figures 18 and 19 show plots of the experimental values of the constants K_1 and K_2 as defined above. Also shown on the graphs are lines representing the equilibrium data given in Kohl and Riesenfeld (1979).

The solid points shown on the figures are from char gasification data, and the open circles are for the New Mexico coal. Figures 18 and 19 suggest that reaction 1 may be at equilibrium while reaction 2 probably is not.

Other Compounds and Elements in Gas Streams

In the previous study of char gasification (Ferrell et al., 1981) the only significant hydrocarbon gas produced was methane. In the gasification of New Mexico coal a large number of hydrocarbon gases are produced. Aliphatics up to butene and butane, and simple aromatic compounds have been detected in the gasifier make gas stream. Figures 20 and 21 plot some of the hydrocarbon emission rates versus the average bed temperature. There is some scatter in the data; however, in general the emission rates appear to increase with increasing temperature.

All compounds analyzed for in the various gas streams are shown in the tables in Appendices C and D. The gas streams were also analyzed for several trace elements; this effort is discussed in a later section of this report.

Compounds Condensed from AGRS Feed Stream

During an integrated run, the gases leaving the PCS system pass through a dehydrator and are then compressed to about 35 Atm. Following the compressor, the gases are cooled to approximately 10°C and pass through a small knockout drum. This drum serves to eliminate pressure fluctuations at the sour gas flow meter and also collects liquids which may condense after compression and cooling.

Figure 18

COMPARISON OF EXPERIMENTAL VALUES OF K1 WITH DATA OF KOHL AND RIESENFELD

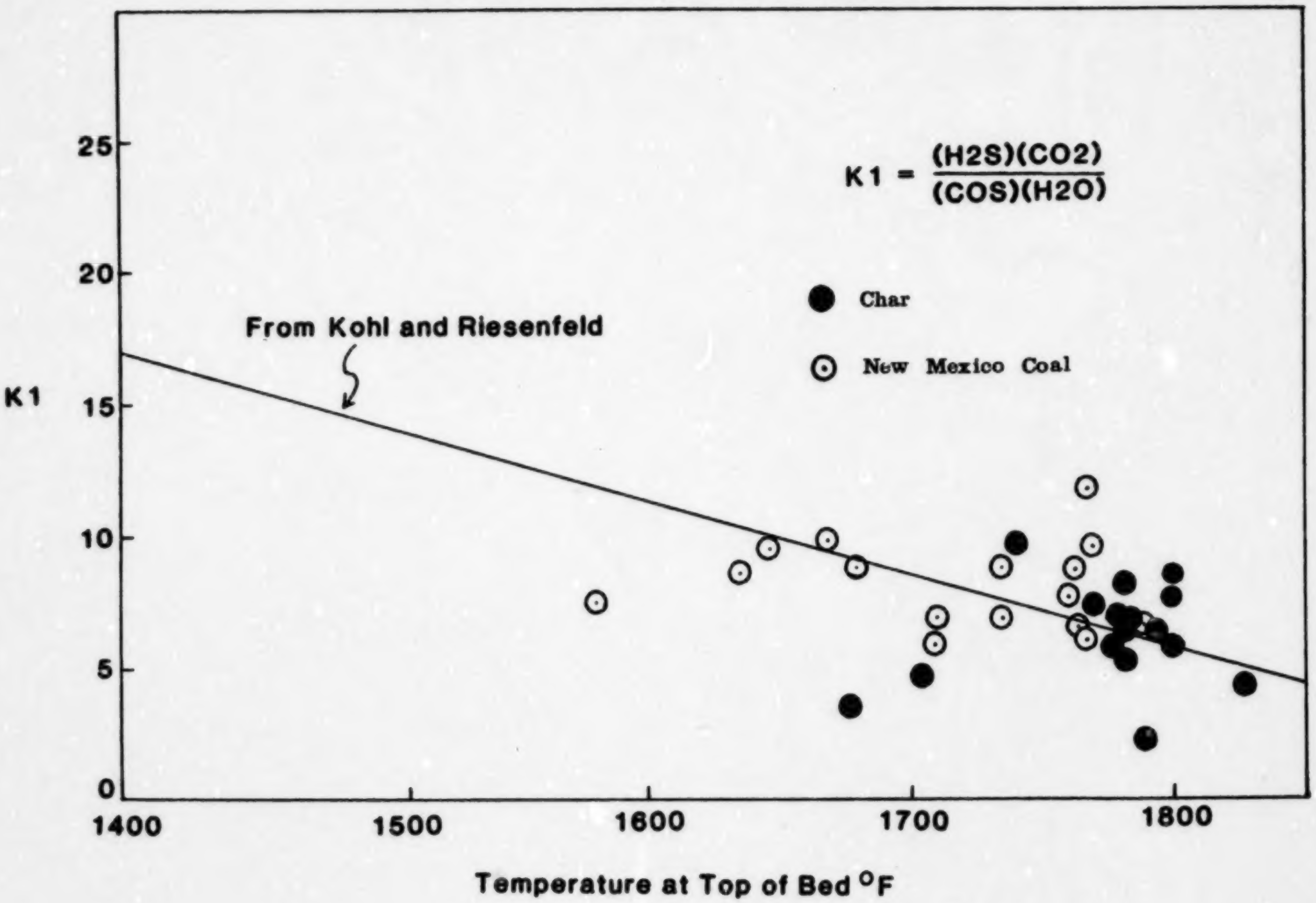


Figure 19

COMPARISON OF EXPERIMENTAL VALUES OF K2
WITH DATA OF KOHL AND RIESENFELD

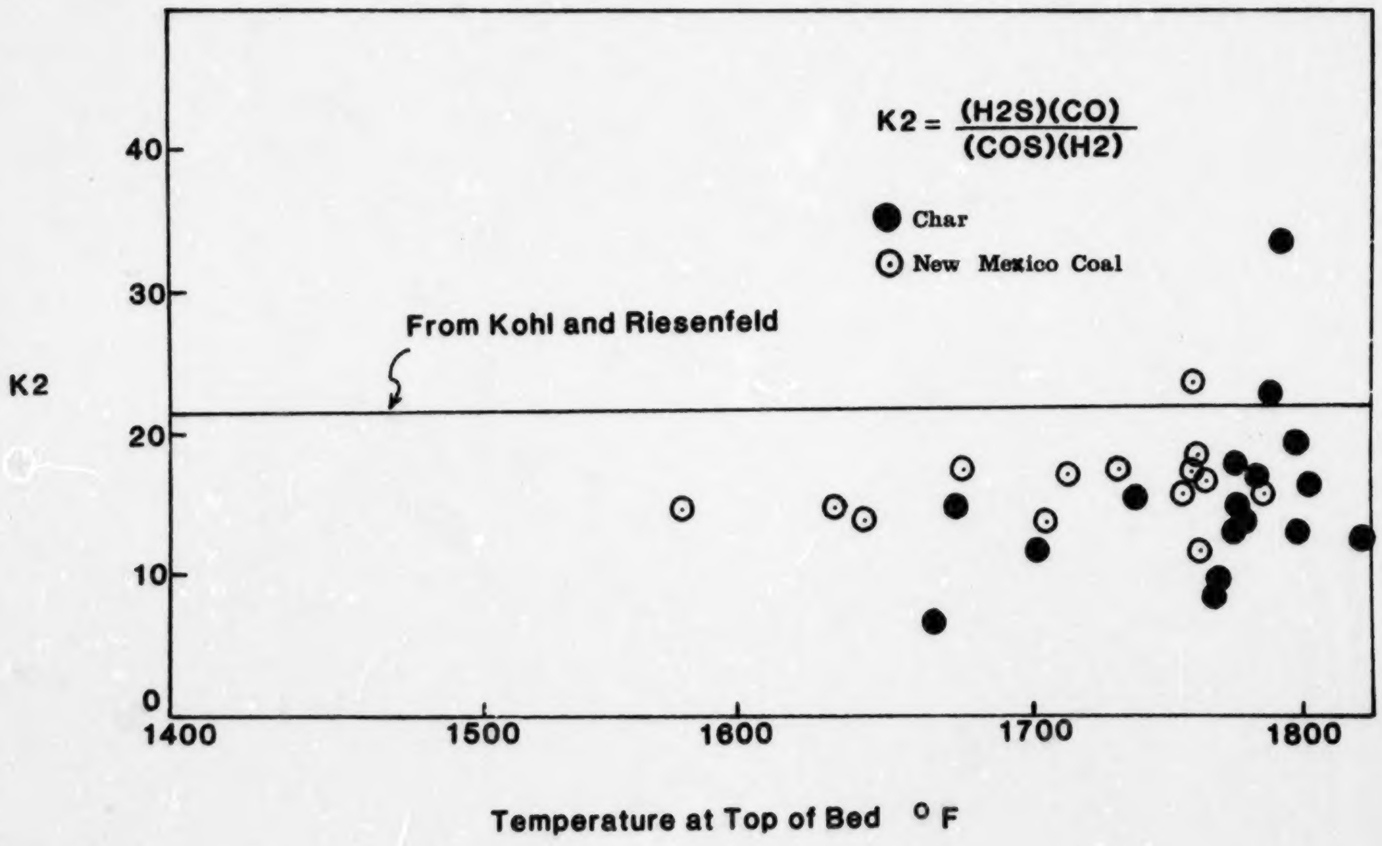


Figure 20
HYDROCARBON EMISSIONS

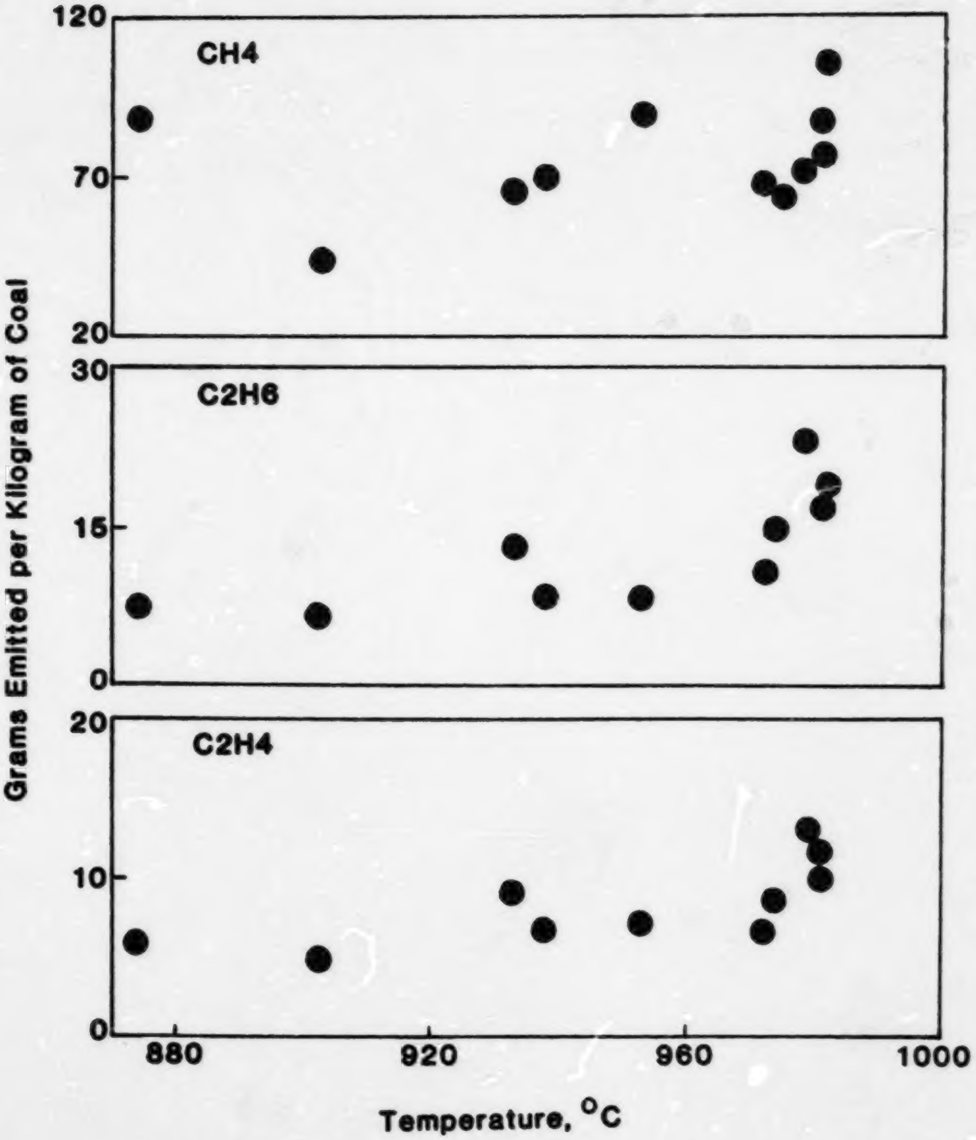


Figure 21

BENZENE AND TOLUENE EMISSIONS

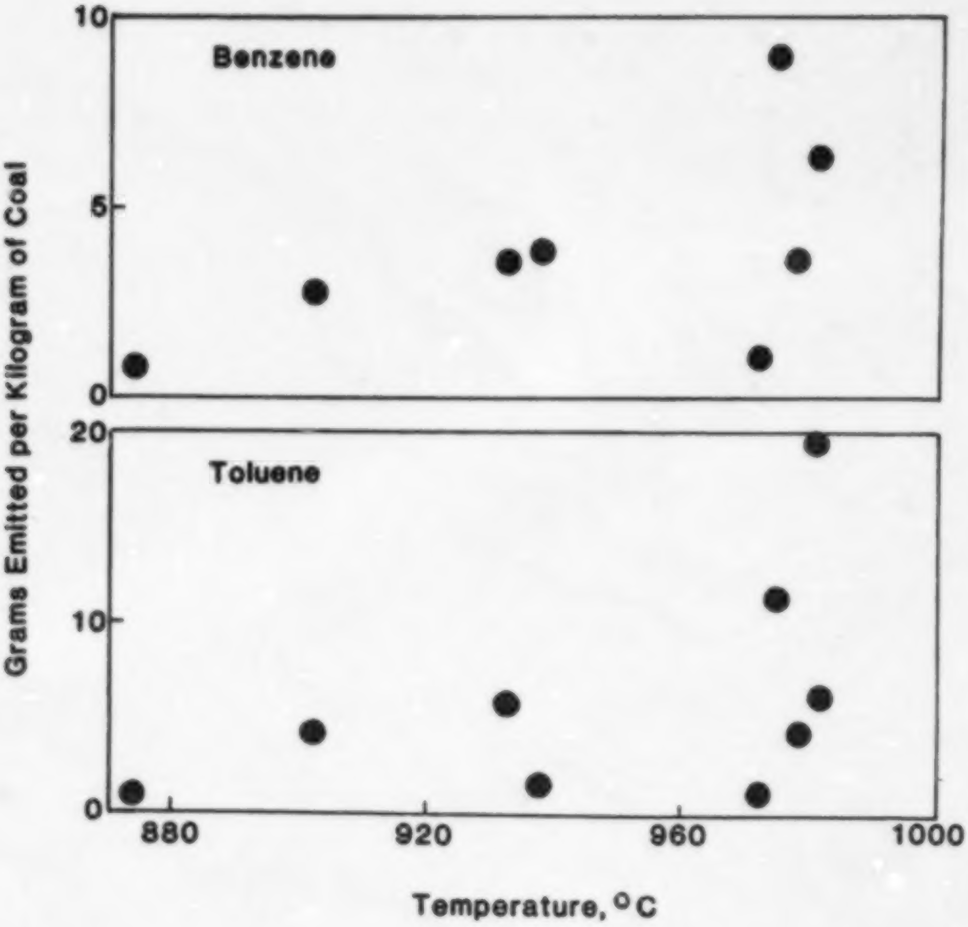


TABLE 3
CONCENTRATIONS AND EQUILIBRIUM CONSTANTS OF MAJOR SULFUR GASES AT TOP OF FLUIDIZED BED

Run No	Top Bed Temp	Mass Recovery %		Gas Concentration							
				ppm Dry		Mole % Wet					
	F	Total	S	H2S	COS	CO	CO2	H2	H2O	K_1	K_2
Western Kentucky Char											
43	1794	104	94	6229	277	16.80	12.36	11.21	43.60	6.4	33.7
44B	1678	99	94	6510	283	6.60	8.82	10.11	57.38	3.5	15.0
45	1671	99	99	3433	266	4.22	6.81	8.27	39.27	2.2	6.6
46	1790	96	97	5478	222	12.77	9.08	13.82	33.14	6.8	22.8
47	1785	97	94	5071	272	13.89	9.86	15.16	29.89	6.2	17.1
48	1778	102	99	6912	312	12.88	10.79	15.77	46.62	5.1	18.1
49	1799	103	91	7052	403	15.42	16.03	13.68	36.25	7.7	19.7
51	1777	104	99	6711	299	10.98	15.11	19.06	41.49	8.2	12.9
53	1771	101	97	8229	343	8.56	13.18	22.42	43.34	7.3	9.2
54	1741	99	101	8736	321	9.92	15.43	17.62	43.03	9.8	15.3
55	1708	102	110	8931	465	9.28	12.61	15.24	50.05	4.8	11.7
56	1800	98	113	8924	410	10.73	12.75	16.98	48.92	5.7	13.8
57	1778	99	107	8098	388	12.74	14.87	18.05	41.92	7.4	14.7
58	1771	103	90	5111	362	11.68	15.80	19.84	38.38	5.8	8.3
59	1803	98	104	8470	306	10.10	14.60	17.15	47.68	8.5	16.3
60	1782	102	121	8887	332	9.26	11.55	18.16	42.48	7.3	13.6
61	1829	96	115	8611	333	8.78	12.20	17.69	49.97	6.3	12.8
New Mexico Coal											
62	1768	102	103	8332	301	7.77	11.63	13.09	53.04	6.07	16.4
63B	1787	99	94	6455	268	11.22	14.16	17.23	44.99	7.58	15.7
64	1760	103	104	6059	255	10.20	15.01	15.31	47.35	7.53	15.8
65	1669	99	108	5743	174	7.57	14.93	14.02	50.12	9.83	17.8
66	1764	99	120	3147	120	11.28	14.80	15.98	44.20	8.78	18.5
68B	1735	98	96	2537	117	12.87	12.44	19.89	39.49	6.83	14.0
69B	1646	97	90	2871	76	7.36	11.91	16.03	47.08	9.56	17.3
70	1737	95	87	2400	76	10.20	12.15	17.97	43.43	8.83	17.9
71B	1769	104	150	3651	118	11.13	12.70	20.15	41.51	9.47	17.1
72	1764	99	122	3344	79	10.02	12.33	17.80	44.60	11.70	23.8
73B	1765	98	57	1275	62	9.71	12.44	18.13	45.05	6.12	11.9
74	1635	95	64	2047	59	7.04	11.51	16.65	47.25	8.45	14.7
76	1679	98	80	2500	78	9.44	12.84	17.25	46.18	8.91	17.5
78	1580	98	86	2439	74	5.88	11.41	13.41	50.00	7.52	14.4
79	1711	101	80	2060	84	9.19	11.40	16.64	46.88	5.96	13.5

A sample of this liquid was collected after run number GO-79 and was analyzed by GC-MS. The mass spectrogram is shown in Figure 22, and the results of compound identification are given in Table 4. While a variety of hydrocarbon compounds were found in this liquid, no aromatic compounds heavier than substituted benzenes were found. This fact, together with results of analyses of the methanol AGRS solvent presented in the following section of this report, indicate that no detectable polynuclear aromatic compounds are in the gases leaving the PCS system.

TABLE 4
COMPRESSOR KNOCKOUT SAMPLE FROM AMI-60/GO-79
PEAK NUMBER FROM FIGURE 22

1. 1-pentene
2. hydrocarbon
3. benzene
4. hydrocarbon
5. toluene
6. cyclo C4-C5
7. hydrocarbon
8. ethyl benzene
9. dimethyl benzene
10. substituted benzene
11. C_8 hydrocarbon
12. C_9 hydrocarbon
13. propyl or ethyl methyl substituted benzene
14. propyl or ethyl methyl substituted benzene
15. 1-decene
16. 2-propyl benzene
17. 1-ethyl-4-methyl benzene

SOLID STREAMS

Proximate and ultimate analyses were carried out on the feed coal, the spent char, and the cyclone fines for all runs made. The results are shown in Tables 5 and 6.

For most of the runs, detailed trace metal analyses were also performed; these results will be presented later in this report. For several of the runs trace metal and ultimate analyses were made on all seive sizes of the coal feed and the spent char. Very little variation in element concentration with sieve size could be found.

The feed coal for run GO-68B was not analyzed, as it was taken from the same drums as the GO-66 feed coal. The GO-66 feed analysis was thus used for GO-68B. For the same reason, the GO-73B feed coal analysis was used for run GO-74. For the runs GO-66 and GO-76, the cyclone was apparently plugged and not working, and the amount of cyclone fines produced was not enough to perform an analysis. For several of the runs the cyclone fines were damp, probably because of condensate formation during system shutdown. The cyclone fines from GO-74 were a wet, tar-like mass, and were not analyzed.

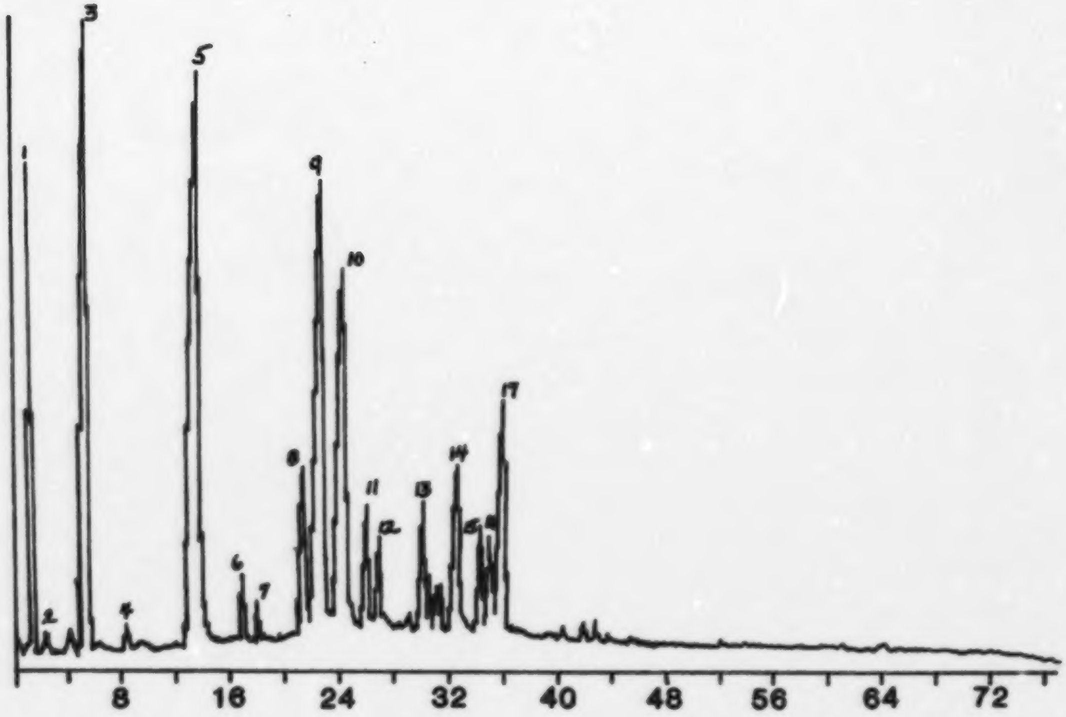


Figure 22

GC/MS SCAN OF COMPRESSOR KNOCKOUT CONDENSATE FOR AMI-60

TABLE 5
PROXIMATE ANALYSIS OF SOLIDS Wt % and Standard Deviation

	GO-66	GO-68B	GO-69B	GO-70	GO-71B	GO-72
Feed						
% Moisture	10.46	——	8.90	10.58	10.39	9.32
Standard Dev.	——	——	0.127	0.021	0.053	0.078
% Vol. Matter	31.78	——	28.17	28.07	31.42	31.70
Standard Dev.	——	——	0.041	0.026	1.008	0.037
% Ash	20.21	——	30.02	28.69	20.51	21.72
Standard Dev.	——	——	1.836	0.009	1.924	0.049
% Fixed Carbon	37.55	——	32.91	32.66	37.68	37.26
Standard Dev.	——	——	1.841	0.035	2.173	0.099
Char						
% Moisture	0.63	1.46	0.31	0.34	0.26	1.09
Standard Dev.	——	——	0.007	0.007	0.122	0.014
% Vol. Matter	9.94	12.48	4.16	3.16	2.92	9.78
Standard Dev.	——	——	0.542	0.895	0.482	0.042
% Ash	72.20	47.07	58.97	91.00	92.80	52.29
Standard Dev.	——	——	0.521	0.507	3.346	0.078
% Fixed Carbon	17.23	38.99	36.56	5.50	4.02	36.84
Standard Dev.	——	——	0.752	1.029	3.383	0.090
Cyclone						
% Moisture	——	1.27	14.34	1.54	0.66	0.60
Standard Dev.	——	——	2.362	0.028	0.007	0.050
% Vol. Matter	——	5.12	9.54	5.93	7.72	4.73
Standard Dev.	——	——	0.282	0.376	0.253	0.133
% Ash	——	69.35	46.81	29.03	51.61	68.34
Standard Dev.	——	——	1.291	2.576	1.946	0.256
% Fixed Carbon	——	24.26	29.31	63.50	40.01	26.33
Standard Dev.	——	——	2.707	2.603	1.962	0.293

TABLE 5 Continued

	GO-73B	GO-74	GO-76	GO-78	GO-79
Feed					
% Moisture	8.81	----	9.46	9.62	9.61
Standard Dev.	0.203	----	0.175	0.028	0.115
% Vol. Matter	31.00	----	32.23	33.23	32.21
Standard Dev.	0.679	----	0.581	0.684	0.270
% Ash	24.17	----	20.59	19.40	21.83
Standard Dev.	1.456	----	1.242	0.083	0.346
% Fixed Carbon	36.01	----	37.72	37.75	36.35
Standard Dev.	1.619	----	1.382	0.690	0.454
Char					
% Moisture	1.26	0.79	0.50	0.37	1.27
Standard Dev.	0.021	0.168	0.062	0.021	0.042
% Vol. Matter	10.10	7.75	6.33	5.73	6.03
Standard Dev.	0.216	1.102	0.179	0.183	0.377
% Ash	62.55	39.40	52.00	58.28	76.07
Standard Dev.	0.259	5.686	2.817	0.184	0.190
% Fixed Carbon	26.09	52.06	41.17	35.62	16.63
Standard Dev.	0.338	5.794	2.823	0.260	0.424
Cyclone					
% Moisture	1.33	----	----	1.06	0.61
Standard Dev.	0.042	----	----	0.007	0.021
% Vol. Matter	4.29	----	----	7.64	5.87
Standard Dev.	0.132	----	----	0.257	1.462
% Ash	65.98	----	----	43.72	60.71
Standard Dev.	0.489	----	----	0.003	0.204
% Fixed Carbon	28.40	----	----	47.58	32.81
Standard Dev.	0.508	----	----	0.257	1.476

TABLE 6: ULTIMATE ANALYSIS OF SOLIDS Wt% and Standard Deviation

	GO-66	GO-68B	GO-69B	GO-70	GO-71B
Feed					
% Carbon	52.55	----	44.71	44.05	50.40
Standard Dev.	----	----	1.110	0.721	2.384
% Hydrogen	4.75	----	3.57	3.63	4.21
Standard Dev.	----	----	0.228	0.007	0.153
% Nitrogen	1.00*	----	0.85	0.96	1.01
Standard Dev.	----	----	0.014	----	----
% Sulfur	0.75	----	0.843	0.794	0.808
Standard Dev.	----	----	0.008	0.005	0.004
% Oxygen	20.74	----	20.01	21.88	23.06
Standard Dev.	----	----	2.158	----	----
Char					
% Carbon	21.72	40.55	31.84	7.53	6.02
Standard Dev.	----	----	0.409	0.269	4.350
% Hydrogen	1.21	1.80	0.49	0.21	0.27
Standard Dev.	----	----	0.056	0.000	0.061
% Nitrogen	0.50*	0.84	0.40	0.50*	0.15
Standard Dev.	----	0.014	0.042	----	0.028
% Sulfur	0.60	0.80	0.515	0.463	0.500
Standard Dev.	----	----	0.020	0.003	0.018
% Oxygen	3.77	8.94	7.79	0.30	0.26
Standard Dev.	----	----	0.666	----	5.488
Cyclone					
% Carbon	----	27.52	----	52.20	42.58
Standard Dev.	----	----	----	0.990	0.969
% Hydrogen	----	0.66	----	0.86	1.15
Standard Dev.	----	----	----	0.010	0.070
% Nitrogen	----	0.60*	0.63	0.60*	0.60*
Standard Dev.	----	----	0.042	----	----
% Sulfur	----	0.32	----	0.287	0.271
Standard Dev.	----	----	----	----	0.022
% Oxygen	----	1.55	----	17.02	3.79
Standard Dev.	----	----	----	----	----

*estimated (See Table 5 for % ash)

TABLE 6 Continued

	GO-72	GO-73B	GO-74	GO-76	GO-78	GO-79
Feed						
% Carbon	52.33	50.01	----	48.70	54.53	52.00
Standard Dev.	0.148	1.805	----	1.891	0.035	0.389
% Hydrogen	4.17	4.14	----	3.45	4.59	4.62
Standard Dev.	0.021	0.234	----	0.127	0.014	0.014
% Nitrogen	1.15	1.06	----	1.00*	1.15	1.10
Standard Dev.	0.028	----	----	----	----	0.078
% Sulfur	0.791	0.814	----	0.828	0.780	0.846
Standard Dev.	0.063	0.020	----	0.010	0.018	0.020
% Oxygen	19.84	19.81	----	25.43	19.55	19.60
Standard Dev.	0.172	----	----	----	----	0.527
Char						
% Carbon	41.34	30.16	49.90	45.65	37.63	8.29
Standard Dev.	0.276	1.096	2.199	0.785	1.435	0.170
% Hydrogen	1.54	0.95	1.25	0.97	0.93	0.34
Standard Dev.	0.057	0.042	0.42	0.000	0.000	0.028
% Nitrogen	0.89	0.50*	0.50*	0.50	0.50*	0.25
Standard Dev.	0.014	----	----	----	----	0.028
% Sulfur	0.666	0.574	----	0.577	0.335	0.536
Standard Dev.	0.007	0.009	----	0.011	0.015	0.014
% Oxygen	3.27	5.27	----	0.30	2.33	14.51
Standard Dev.	0.293	----	----	----	----	0.258
Cyclone						
% Carbon	52.26	28.55	----	----	44.95	34.02
Standard Dev.	0.219	1.980	----	----	2.199	0.205
% Hydrogen	4.00	0.57	----	----	1.11	0.84
Standard Dev.	0.085	0.163	----	----	0.042	0.028
% Nitrogen	0.32	0.60*	----	----	0.60*	0.88
Standard Dev.	0.021	----	----	----	----	0.127
% Sulfur	0.221	0.219	----	----	0.440	0.302
Standard Dev.	0.000	0.001	----	----	0.001	0.004
% Oxygen	----	4.08	----	----	9.18	3.25
Standard Dev.	----	----	----	----	----	0.317

*estimated (See Table 5 for % ash)

Determination of nitrogen was not done for all runs, as the analysis is highly time consuming and the amount of nitrogen in the coal is small. In Table 6 average values of nitrogen content are used as estimates where no nitrogen analysis was performed.

In general, the ultimate analysis of the spent char correlates with gasifier run conditions. For example, higher temperatures result in higher carbon conversions and a lower carbon content in the spent char.

TAR

Tar samples were collected from runs GO-69B, GO-70, GO-76, and GO-78, and were analyzed by the Research Triangle Institute, Research Triangle Park, North Carolina, under a separate contract with EPA. The results of these analyses are given in Tables 7-9, and Figures 23 and 24.

For runs 69B, 70, and 76, tar samples were collected from the PCS tank. After the completion of a run, the PCS tank was emptied by pumping the contents of the tank out through a filter followed by a char bed to remove dissolved organic compounds before discharging to the sewer system. The tar samples from the PCS tank were obtained from material collected on the filter, and contained both tar and particulates, as well as some water. The tar was separated from the particulates by dissolving in methylene chloride. For runs 76 and 78, tar samples were taken from the cold trap at the sample train. As discussed elsewhere in this report, the cold trap collects all condensed water, tar, and particulates for a period during the steady state portion of a run. It is believed that the tar collected from the cold trap provides better defined samples than that collected from the PCS tank. For comparison, samples from both locations were taken for run GO-76, and both analyses are shown in Table 8. The sample from the cold trap appears to be somewhat more concentrated in the compounds analyzed for, although the differences are not very significant, either in compound concentrations or in the tar partitioning results shown in Table 7.

The tars were subjected to a solvent partitioning scheme in order to separate them into groups of compounds of varying polarities. The groups were then quantified as to their weight percent contribution to the total tar composition. The partitioning results are shown in Table 7. In addition to the partitioning analysis, the tars were analyzed for polynuclear aromatic hydrocarbons and organic sulfur compounds. The PNA's were analyzed by glass capillary gas chromatography with a flame ionization detector. A chromatogram of the GO-69 PNA's is shown in Figure 23.

The sulfur-containing species were analyzed by gas chromatography with a flame photometric detector. A chromatogram showing the GO-69 sulfur species is given in Figure 24.

Figure 23

CAPILLARY GC SCAN OF TAR FOR PNA COMPOUNDS

GO-69

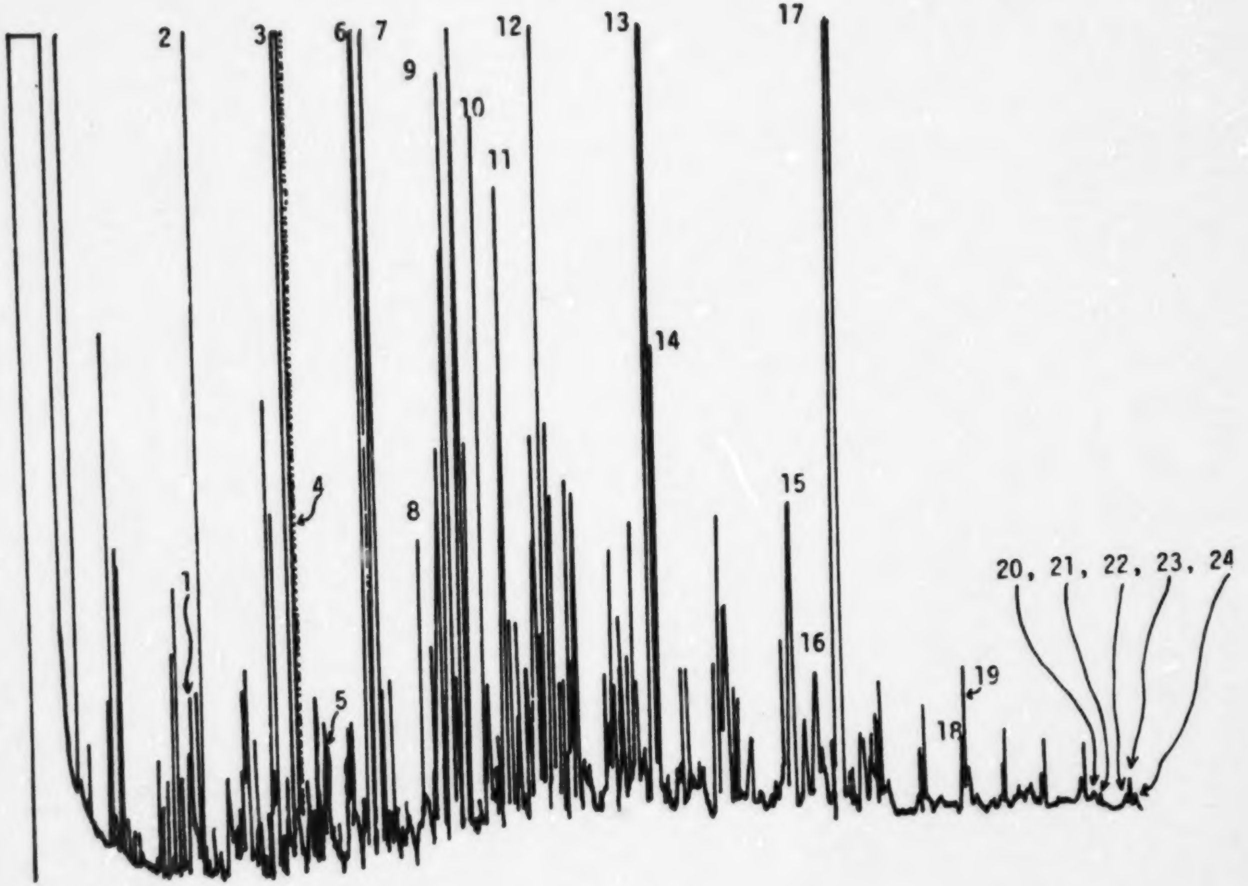


Figure 24

CAPILLARY GC SCAN OF TAR FOR SULFUR COMPOUNDS
GO-69

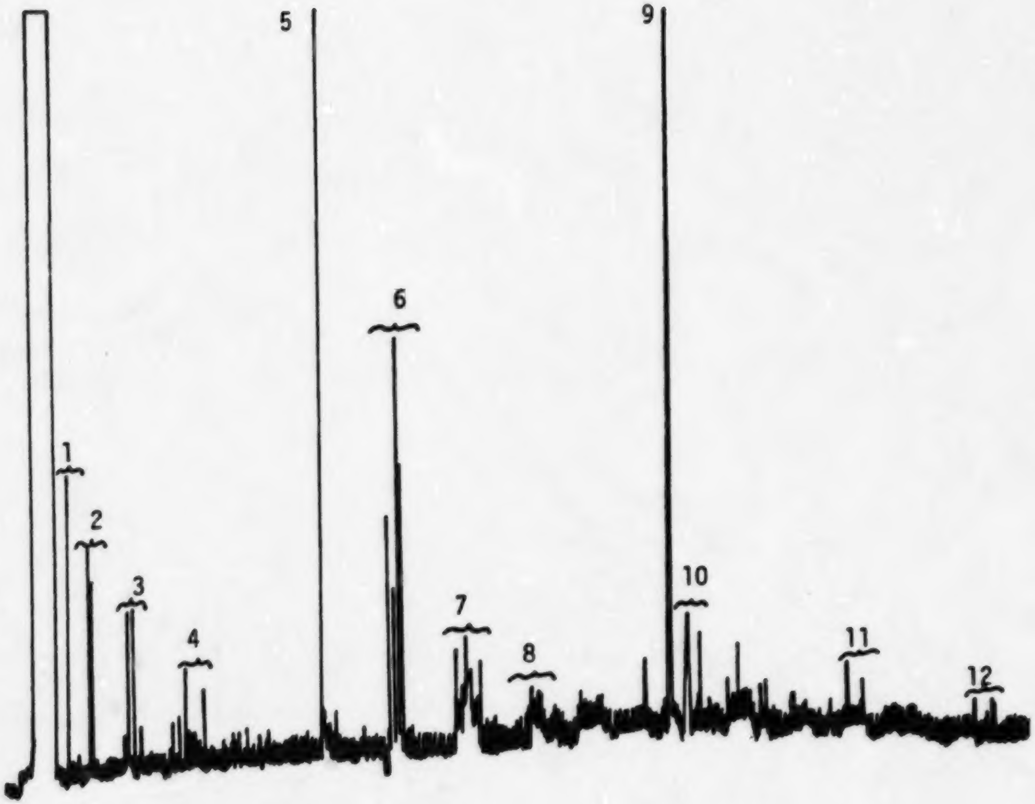


TABLE 7
TAR PARTITION RESULTS Wt %

	GO-69B PCS	GO-70 PCS	GO-76 Trap	GO-76 PCS	GO-78 Trap
Acids	10.9	34.7	16.5	11.2	17.29
Bases	20.9	27.5	4.7	6.7	6.05
TOTAL NEUTRALS	68.3	37.7	78.8	80.1	76.66
Non polar	25.1	5.5	24.7	30.0	11.53
PNAs	36.0	26.7	10.7	11.5	26.85
Polar	7.2	5.5	15.3	15.2	16.45
Cyclohexane Insolubles	--	—	28.1	23.4	21.83

TABLE 8
CAPILLARY GC TAR ANALYSES Wt %

Peak No Figure 23		GO-69 PCS	GO-76 Trap	GO-76 PCS	GO-78 Trap
1	Phenol	0.15	———	———	———
2	Indene	0.87	———	———	———
3	Naphthalene	3.50	2.11	1.30	2.10
4	Benzothiophene	0.13	0.09	0.06	0.08
5	Quinoline	0.08	0.16	0.09	0.13
6	2-Methylnaphthalene	1.60	0.79	0.60	0.97
7	1-Methylnaphthalene	1.10	0.52	0.37	0.81
8	Biphenyl	0.36	0.16	0.14	0.28
9	Acenaphthylene	1.50	0.71	0.53	0.60
10	Acenaphthene	0.57	0.34	0.30	0.26
11	Dibenzofuran	0.74	0.53	0.46	0.53
12	Fluorene	1.00	0.53	0.51	0.43
	Dibenzothiophene	0.09	0.07	0.08	0.09
13	Phenanthrene	1.30	0.62	0.67	0.47
14	Anthracene	0.73	0.38	0.32	0.49
15	Fluoranthene	0.45	0.36	0.32	0.23
16	Pyrene	0.32	0.26	0.25	0.17
17	Benzo(a)anthracene	0.09	0.16	0.07	0.05
18	Chrysene	0.14	0.13	0.09	0.04
19	Triphenylene	0.14	0.06	0.03	0.02
20	Benzo(b)Fluoranthene	0.04	0.11	0.05	0.013
21	Benzo(k)Fluoranthene	0.02	0.06	0.01	0.007
22	Benzo(e)Pyrene	0.05	0.05	0.01	0.007
23	Benzo(a)Pyrene	0.04	0.11	0.03	0.015
24	Perylene	0.02	0.05	0.01	0.01
	Total Wt %	15.03	8.36	6.30	7.802

The analysis of the tars indicate that a significant amount of PNA's are in the gas stream as it leaves the reactor, and emerge primarily in the tar stream condensed by the venturi scrubber. It appears that compounds with boiling points higher than that of naphthalene are not present in the gas stream past the PCS system.

TABLE 9
QUANTITATIVE ANALYSIS OF SULFUR SPECIES Wt %
Tar Sample, Run No. GO-69B

Peak No Figure 24	Compound	Concentration
1	thiophene	0.01
2	methylthiophenes	0.02
3	C_2-thiophenes	0.03
4	C_3-thiophenes	0.03
5	benzothiophene	0.13
6	C_1-benzothiophenes	0.05
7	C_2-benzothiophenes	0.06
8	C_3-benzothiophenes	0.05
9	dibenzothiophenes	0.09
10	napthothiophenes	0.08
11	phenanthrothiophenes	0.06
12	naphthobenzothiophenes	0.09
	Total	0.70

WASTEWATER

Water samples were collected from both the PCS tank and from the sample train. Samples from the PCS tank were collected after the completion of a run, and thus represent the accumulaton of material during the times of startup, steady state operation, and shutdown. Water samples labeled as trap water were taken from the sample train, either from the condensate receiver or from the cold trap after its removal at the end of the run. Trap water samples from either location of the sample train are essentially identical, and are from the steady state portion of a run.

The water sample analyses shown in Table 10 were carried out by the Research Triangle Institute. The location of the sample is also indicated as either PCS or Trap. As expected, concentrations in the trap water are substantially higher than those in the PCS tank water. The water samples from the trap provide a better representation of the conditions at steady state at a well defined reactor operating condition.

These samples were analyzed by high-performance liquid chromatography (HPLC) for phenolics. The sample preparation consisted of filtering to remove particulates prior to direct injection into the HPLC. The results are not reported as specific phenolic compounds, but are categorized as phenols, cresols, and xylenols. In addition, the samples were analyzed for total organic extractables. A methylene chloride extraction was performed and the extract evaporated to dryness in order to determine the weight percent of organic extractables in the sample.

TABLE 10
WATER ANALYSES mg/l

	GO-69B PCS	GO-70 PCS	GO-76 Trap	GO-76 PCS	GO-78 Trap
phenol	870	637	1250	220	1584
cresol	690	398	693	166	783
xylenols	230	881	161	97	510
organic extractables	1620		2040	460	1900

In addition, both the trap water and water from the PCS tank were analyzed by the methods described earlier, and these results are shown in Tables 11 through 14. Table 11 shows average values for all of the runs reported on here, and is intended to show the general levels of concentrations found as well as the differences between the two kinds of samples collected. Tables 12, and 13 show the details of all individual analyses performed. The tables show significant differences between the RTI and the NCSU analyses for phenolics. The NCSU values are adequate for evaluating trends, but are believed to be low in magnitude. Methods are currently under development to improve this analytical method.

Table 14 shows the data of Table 13 normalized to show the rate of evolution of the various species in milligrams per kilogram of coal fed to the gasifier. The data are plotted versus the average bed temperature in Figures 25 through 28. No clear trends with temperature are shown by the plots, indicating that for the temperature range covered the reactor temperature has little effect on the emission rates of wastewater species. Some of the scatter in Figures 25 through 28 may be due to analysis inaccuracies. Work is currently being done to refine all wastewater analysis methods.

Figure 25

REACTOR EMISSIONS IN TRAP WATER

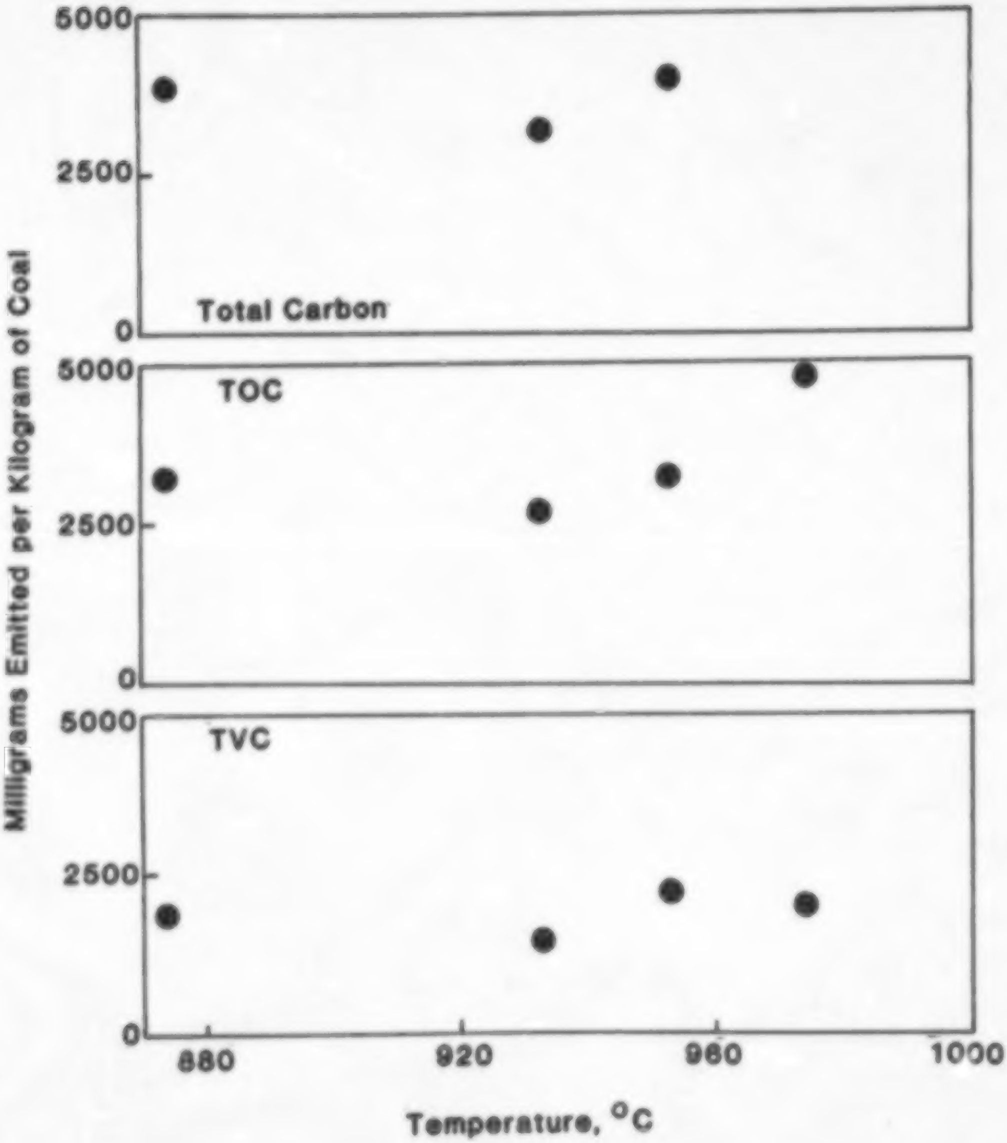


Figure 26
REACTOR EMISSIONS IN TRAP WATER

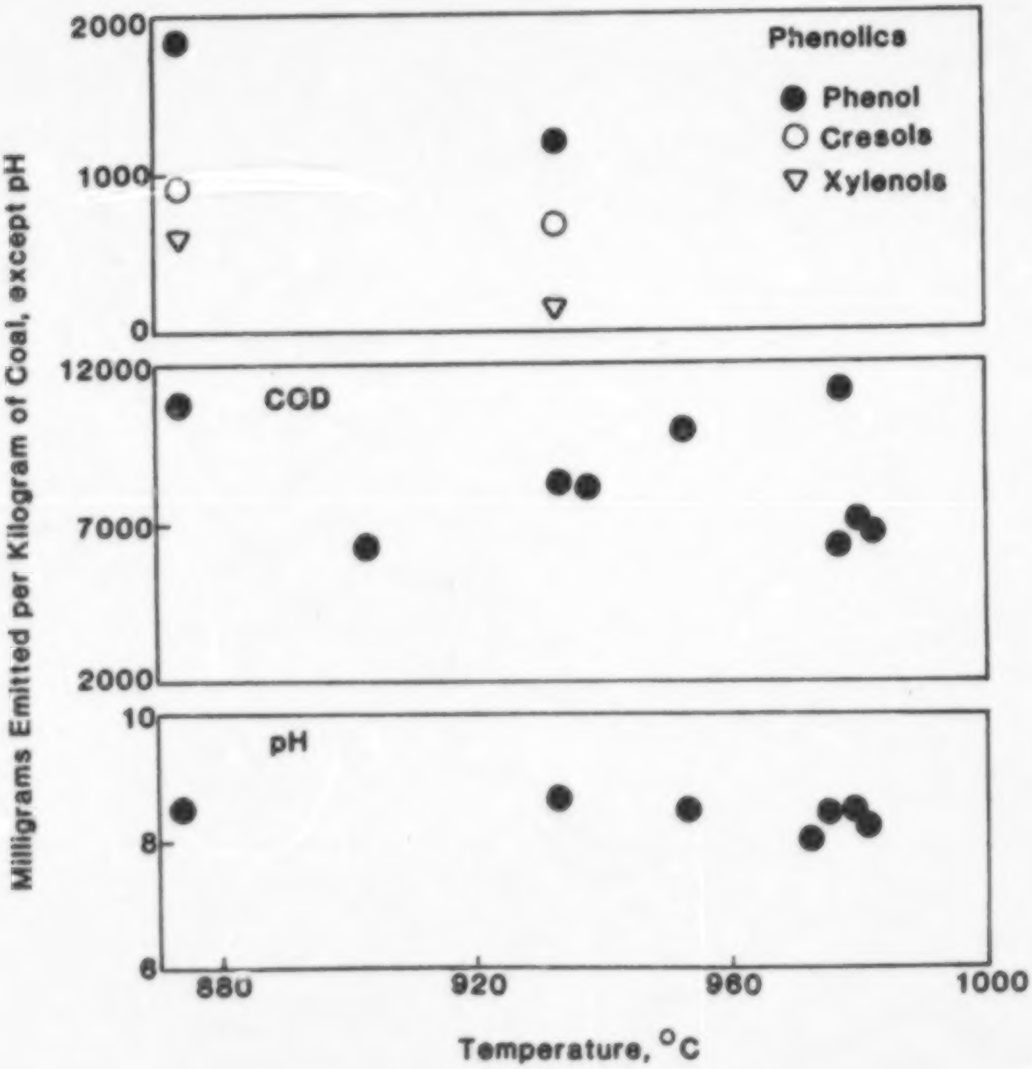


Figure 27

REACTOR EMISSIONS IN TRAP WATER

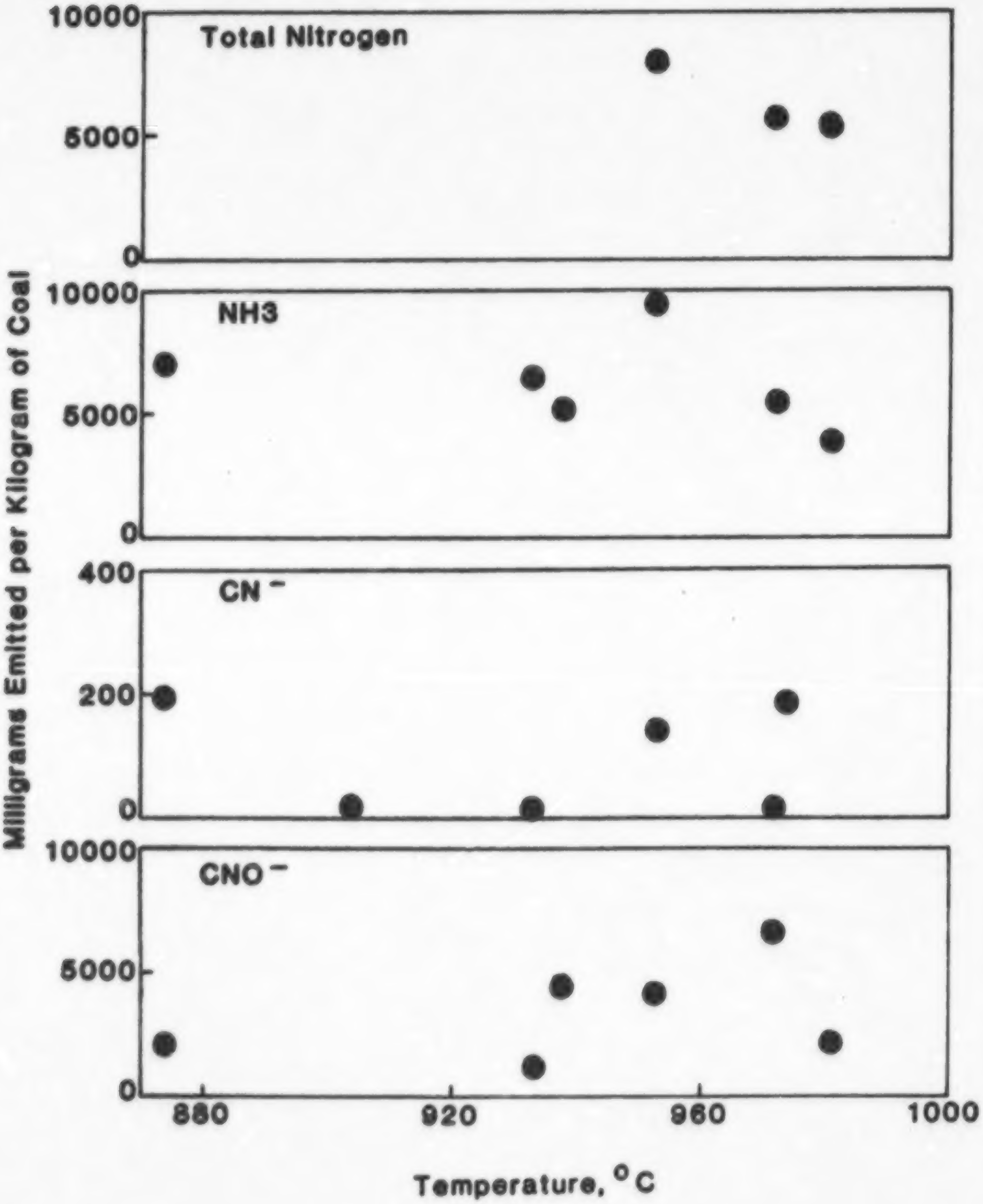


Figure 28

REACTOR EMISSIONS IN TRAP WATER

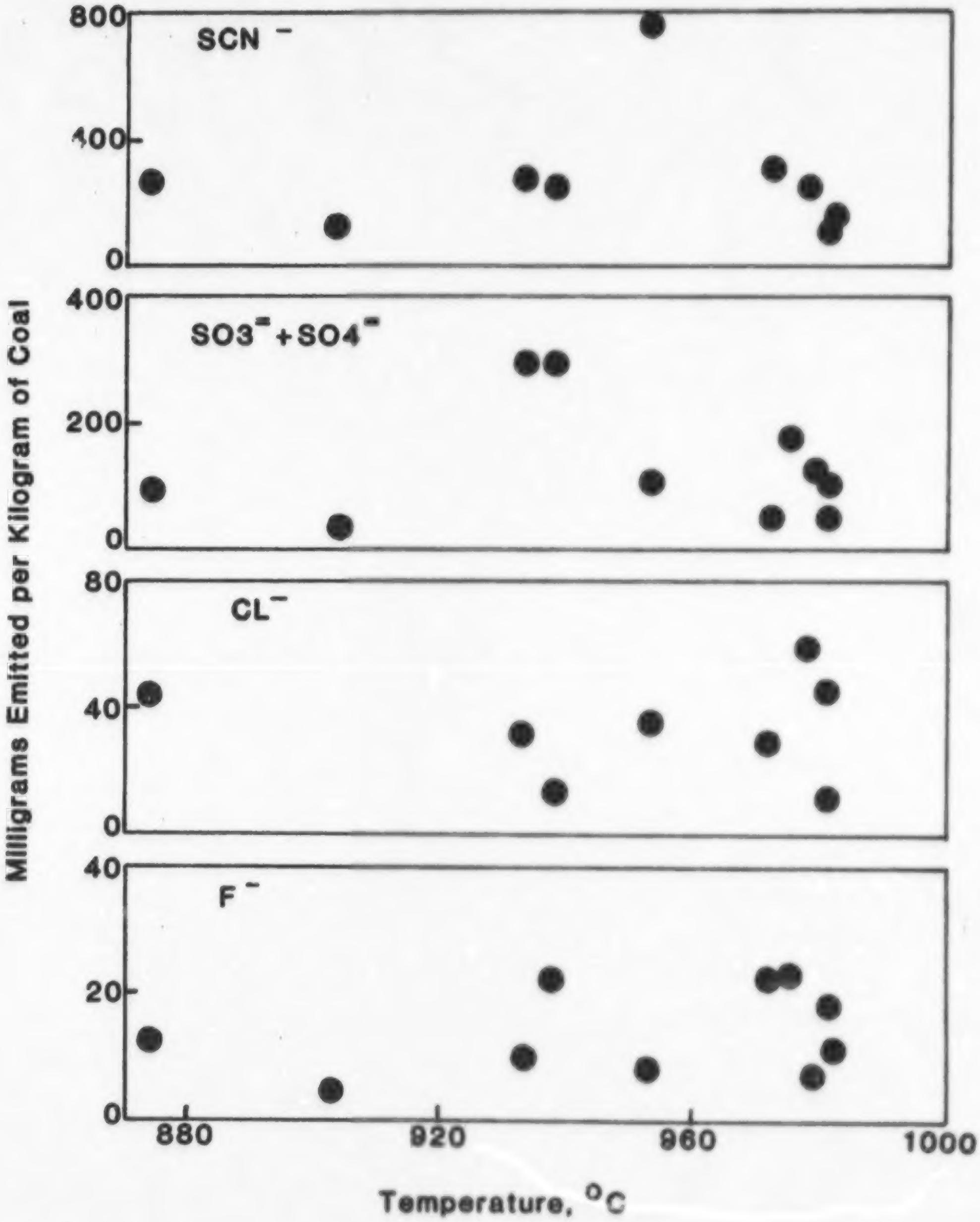


TABLE 11
WATER ANALYSIS FOR ALL RUNS mg/l except pH
Values Shown are Averages or Minimum-Maximum Values

	PCS water	Trap water
Ammonia	700	6,000
Carbon	725	3,200
Chloride	20	40
COD	1,500 - 3,000	6,000 - 10,000
Cyanate	500	2,000 - 5,000
Cyanide	45	25 - 200
Fluoride	5	10
Nitrogen	600	6,000
pH	7.7	8.5
Phenolics	200 - 400	600 - 1,100
Sulfate	35	40 - 300
Sulfite	15	40
Thiocyanate	50	250
TOC	400 - 600	2,600
TVC	325	1,500

TABLE 12
SUMMARY OF PCS TANK WATER ANALYSIS mg/l except pH

	(10%)* GO-62	(30%)* GO-63	(50%)* GO-64	(50%)* GO-65	GO-66	GO-68	GO-68B
Ammonia	272.2	298.1	161.4	311.1	400.7	307.2	
Carbon						638	
Chloride							
COD	628	864	740	759		605	628
Cyanate	366.4	369.7	211.6		543.3	390.7	
Cyanide							
Fluoride							
Nitrogen	277.8		170.4	320.9	374.7		
pH						7.7	
Phenolics	1.7	8.5	5.1	7.4	19.3	20.7	250
Sulfate							
Sulfite							
Sulfur							
Thiocyanate		27.6	16.5		41.5	25.4	
TOC						605	1000
TVC						263	

* Percentages refer to % coal (all other runs 100% coal)

	GO-69B	GO-71B	GO-72	GO-73	GO-74	GO-76	GO-77
Ammonia		798.7				721	
Carbon						890	640
Chloride				22	16.5	17	18
COD	3800	1563	1266	2532	1772	1810	2250
Cyanate		1011				47	
Cyanide		65.5			24	21	
Fluoride				5.8	3.5	3	3
Nitrogen		795.2					
pH						5.7	
Phenolics	400.2	339.5	201.5	178	188	141	76
Sulfate				37	35.3	36	32
Sulfite				14	9.6	14	16
Sulfur							
Thiocyanate		68.7	31.3	52.8		31.7	
TOC						600	420
TVC						380	360

TABLE 13

SUMMARY OF TRAP WATER ANALYSIS Concentrations in mg/l except pH

	(10%)* GO-62	(30%)* GO-63	(50%)* GO-64	(50%)* GO-65	GO-66	GO-68B	GO-69B	GO-70
Ammonia							5633	5795
Carbon	960							
Chloride							14	31
COD						41.5	8900	6667
Cyanate							5014	7167
Cyanide						265		10.6
Fluoride						31.4	24.1	22.6
Nitrogen								6096
pH						8.48		8.0
Phenolics		41.8					1686	879.4
Sulfate						191.2	305	41.4
Sulfite						64.5	18.5	11.4
Thiocyanate							279.2	330.4
TOC	540					6800		
TVC	350					2850		

* Percentages refer to % coal (all other runs 100% coal)

	GO-71B	GO-72	GO-73	GO-74	GO-76	GO-78	GO-79
Ammonia	3966				6804	6065	6886
Carbon					3300	3380	2920
Chloride	45.7	9.5	49		33.2	38	26.5
COD	6563	6228	9367	9982	8600	9350	7510
Cyanate	2330				1255	1749	3075
Cyanide				13	22	167	107
Fluoride	10.8	16.0	5.6	5.5	10	10	6
Nitrogen	5391						5874
pH		8.3	8.5		8.7	8.5	8.5
Phenolics	916.9	1127	551	827	791	772	597
Sulfate	72.5	13.5	39	44.2	280	27.5	31
Sulfite	30.3	33.7	68	11.4	28	55	45
Thiocyanate	147.1	103.3	214	195	290	233	581
TOC					2800	2760	2360
TVC					1500	1630	1590
RTI analysis							
Phenol					1250	1584	
Cresol					693	783	
Xylenols					161	510	
Organic Extractables					2040	1900	

TABLE 14
SUMMARY OF EMISSIONS FROM TRAP WATER ANALYSIS
Milligram per Kilogram of Coal Fed except pH

	(10%)* GO-62	(30%)* GO-63	(50%)* GO-64	(50%)* GO-65	GO-66	GO-68B	GO-69B	GO-70
Ammonia							5177	5503
Carbon	1404							
Chloride							13	29
COD						30	8180	6331
Cyanate							4608	6806
Cyanide						190		10
Fluoride						23	22	22
Nitrogen								5789
pH						8.48		8.0
Phenolics		44					1550	835
Sulfate						137	280	39
Sulfite						46	17	11
Thiocyanate							257	314
TOC	790					4871		
TVC	512					2042		

* Percentages refer to % coal (all other runs 100% coal)

	GO-71B	GO-72	GO-73	GO-74	GO-76	GO-78	GO-79
Ammonia	4024				6586	7051	9455
Carbon					3194	3929	4010
Chloride	46	11	59		32	44	36
COD	6658	6927	11211	6330	8324	10869	10312
Cyanate	2364				1215	2033	4222
Cyanide				8	21	194	147
Fluoride	11	18	7	4	10	12	8
Nitrogen	5469					8066	
pH		8.3	8.5		8.7	8.5	8.5
Phenolics	930	1254	660	524	766	898	820
Sulfate	74	15	47	28	271	32	43
Sulfite	31	38	81	7	27	64	62
Thiocyanate	149	115	256	124	281	271	798
TOC					2710	3209	3241
TVC					1452	1895	2183
RTI Analysis							
Phenols					1210	1841	
Cresols					671	910	
Xylenols					156	593	
Organic Extractibles					1975	2209	

TRACE METAL BALANCE RESULTS

Results and Discussion

Summaries of concentrations and mass balances for arsenic, lead, and mercury are given in Tables 15-17. The closures on the balances are clearly unsatisfactory for all three elements. The ensuing paragraphs summarize the principal results shown in these tables, and suggest possible reasons for the inadequacies in the data and steps that might be taken to remedy them.

Closures on arsenic consistently vary between 35% and 70%, suggesting that a significant fraction of this substance is passing undetected from the system, either in the gas phase or adsorbed on fine particles that are not trapped by the cold trap or impingers. Similar results are obtained for lead, for which the closures never exceeded 34%, indicating a higher volatility for this element. However, this picture might change when the analyses for the last two runs in the table have been completed, since only in one of the first four runs were all effluent streams analyzed.

The problem with mercury is reproducibility, rather than failure to detect a portion of the total emitted element. The quantity of this element appearing in the trapped tar and solids varies dramatically from one run to another. In some instances the apparent amount of mercury in one or the other of these streams exceeds the quantity fed in with the coal.

The conclusions that may be derived from these studies at the present time may be summarized as follows:

1. As earlier studies have indicated, all three elements are volatile, and can be expected to be present in significant amounts in the gas that exits the cyclone separator. Mercury is the most volatile of the three, followed in order of decreasing volatility by lead and arsenic.

2. Of the quantities of the elements that enter the gasifier in the feed coal, roughly 20-50% of the arsenic is retained in the spent char and the cyclone dust. The comparable figure for lead is 10-20%, and only 5-15% of the entering mercury is retained. While we cannot yet say how much of each of these elements is likely to be recovered by the various gas cleaning processes, it is clear that a substantial fraction of the amounts that enter will be present in the various effluent streams from the pilot plant downstream of the gasifier.

3. As might be expected, the gasifier temperature has a noticeable effect on the level of volatilization of the elements. Of the six runs for which data are given, the lowest average bed temperature was 873°C in Run GO-78, with the temperatures in all other runs being significantly higher. The retention of arsenic in the spent char and cyclone dust was 48% at the low temperature, as contrasted with 13-36% at the higher

temperatures. Lead data for GO-78 are not yet available, but the 13% retention at the high temperature in GO-70 is significantly lower than the values at lower temperatures. At the lowest temperature, 36% of the mercury was retained, while at the higher temperatures only 4-15% was retained.

4. The concentrations of arsenic in the cyclone dust and the solids trapped in the cold trap are almost invariably much higher than those in the feed coal. This suggests the occurrence of a recondensation process, in which arsenic volatilized in the gasifier readsorbs on fine elutriated particles. A better mass balance closure on this element might therefore be obtained if a fines filter more efficient than the cold trap steel wool were used in the sampling line.

5. The preliminary results for lead indicate the same concentration effect as was observed for arsenic. Trapping all fines and perfecting the impinger system is even more critical for lead than for arsenic, in view of the apparently higher volatility of this element.

6. Most of the mercury entering the gasifier is volatilized. Although the scatter in the data for this element makes it impossible to draw quantitative conclusions, it seems clear that substantial amounts of the element are recovered in the cold trap, either with the tar or the solids fraction or both. It will therefore be necessary to quantify the amounts of these two fractions more precisely than is done now, to avoid major errors when the cold trap condensate amount is scaled up to determine the total flow rate in the cyclone exit gas.

7. The gold amalgamation columns appear to be working well. When the cold trap data are made more reproducible, the combination of the cold trap and the gold columns should yield satisfactory mercury balance closures.

8. The cyclone dust shows an increasing element concentration with decreasing particle size, but the effect is slight.

TABLE 15
RESULTS FOR ARSENIC

Run No	TOTAL IN	OUTLET STREAMS						TOTAL OUT (% recovery)
	Feed Coal	Spent Char	Cyclone Dust	Trap Tar	Trap Solid	Trap Water	Gas	
GO-69B	9.1	8.1	12.3	6.4	*	1.63	-	
(938°C)	230	81	*	8	*	38	-	127
		36%	*	3%	*	17%	-	56%
GO-70	17.3	11.2	22.5	8.5	12.5	0.55	-	
(972°C)	380	67	28	16	19	11	-	142
		18%	7%	4%	5%	3%	-	37%
GO-71B	2.4	0.4	6.7	2.1	4.3	0.03	-	
(981°C)	50	2	8	*	6	2	-	18
		4%	17%	*	13%	1%	-	35%
GO-76	4.0	3.5	*	2.1	11.8	0.26	-	
(932°C)	91	21	*	2	8	6	-	37
		23%	*	2%	9%	7%	-	41%
GO-78	3.5	3.6	9.8	2.4	7.1	0.19	-	
(873°C)	66	22	10	4	1	4	-	41
		33%	15%	6%	1%	7%	-	61%
GO-79	4.2	2.3	6.8	2.7	11.8	0.07	-	
(954°C)	69	5	3	7	21	3	-	40
		8%	5%	10%	31%	4%	-	58%

1. First row for each run gives concentrations in ppm
2. Second row for each run provides mass flows in mg/h
3. Third row for each run indicates percent of amount in feed coal

TABLE 16
RESULTS FOR LEAD

Run No	TOTAL IN	OUTLET STREAMS						TOTAL OUT (% recovery)
	Feed Coal	Spent Char	Cyclone Dust	Trap Tar	Trap Solid	Trap Water	Gas	
GO-69B	9.5	5.2	10.9	3.4	*	0.24	-	
(938°C)	236	52	*	4	*	5	-	61
		22%	*	2%	*	2%	-	26%
GO-70	5.2	1.3	5.9	9.1	3.6	0.05	-	
(972°C)	114	8	7	17	5	1	-	39
		7%	6%	15%	5%	1%	-	34%
GO-71B	5.5	1.7	8.1	7.0	5.2	0.02	-	
(981°C)	114	10	10	*	8	<1	-	29
		9%	9%	*	7%	<1%	-	26%
GO-76	5.8	4.0	*	2.0	14.5	0.09	-	
(932°C)	134	24	*	2	10	2	-	38
		18%	*	1%	7%	2%	-	28%
GO-78	LEAD ANALYSES NOT YET COMPLETE							
GO-79	LEAD ANALYSES NOT YET COMPLETE							

1. First row for each run gives concentrations in ppm
2. Second row for each run provides mass flows in mg/h
3. Third row for each run indicates percent of amount in feed coal

TABLE 17
RESULTS FOR MERCURY

Run No	TOTAL IN	OUTLET STREAMS						TOTAL OUT (% recovery)
	Feed Coal	Spent Char	Cyclone Dust	Trap Tar	Trap Solid	Trap Water	Gas	
GO-69B	0.109	0.024	0.187	0.052	*	0.007	0.290^{+}	
(938°C)	2.7	0.24	*	0.06	*	0.16	0.32	0.79
		9%	*	2%	*	6%	12%	29%
GO-70	0.013	0.0019	0.0041	0.093	0.189	0.002	0.104^{+}	
(972°C)	0.20	0.01	0.01	0.18	0.29	0.04	0.12	0.65
		4%	2%	62%	100%	14%	43%	225%
GO-71B	0.137	0.052	0.086	*	*	–	0.52^{+}	
(981°C)	2.9	0.31	0.11	*	*	0.02	0.68	1.12
		11%	4%	*	*	1%	24%	39%
GO-76	0.042	0.023	*	0.29	0.98	0.002	*	
(932°C)	1.0	0.14	*	0.28	0.66	0.05	*	1.13
		14%	*	29%	68%	5%	*	117%
GO-78	0.058	0.048	0.054	1.47	5.33	0.003	0.267^{+}	
(873°C)	1.1	0.29	0.09	2.36	0.67	0.08	0.25	3.74
		27%	9%	218%	62%	7%	23%	346%
GO-79	0.111	0.023	0.045	0.228	0.421	0.0004	*	
(954°C)	1.8	0.07	0.02	0.60	0.76	0.02	*	1.45
		3%	1%	33%	42%	<1%	*	80%

1. First row for each run gives concentrations in ppm
2. Second row for each run provides mass flows in mg/h
3. Third row for each run indicates percent of amount in feed coal

COAL GASIFICATION RESULTS

Gasifier runs with New Mexico subbituminous coal were commenced by feeding mixtures of the subbituminous coal and a devolatilized Western Kentucky coal char used in previous studies. This was done in order to evaluate the ability of the system to handle the tars associated with the coal feedstock. Runs GO-62 through GO-65 used 10, 30, 50, and 50 weight percent subbituminous coal respectively, with the balance being char. The success of these runs indicated that 100% New Mexico subbituminous coal could be used as a feedstock. For runs GO-66 through GO-79 the feed was 100% coal. Results for all runs are included in this report; however, the runs with 100% coal as the feed form the data base used in the plots and modeling work that follow.

A summary of the operating conditions and experimental results is given in Table 18 for all runs. In processing the data for these runs, the purge nitrogen flow rate was adjusted to close the nitrogen balance. This was done to correct for purge nitrogen leaks in the system. All other tabulated results are based on actual operating and analytical data.

TABLE 18
SUMMARY OF RUNS FOR GASIFIER-AGRS
USING NEW MEXICO COAL AND METHYL ALCOHOL

Gasifier	GO-62	GO-63B	GO-64	GO-65	GO-66
Date	8/20/80	9/13/80	9/25/80	10/ 2/80	10/22/80
Avg Bed Temp °F	1805	1816	1802	1707	1799
Pressure psig	102	103	103	103	104
Coal Feed lb/hr	45.0	39.0	41.4	48.3	42.6
% Coal	10	30	50	50	100
Steam Feed lb/hr	56.9	56.5	57.3	59.9	57.3
Steam/Carbon Ratio	1.09	1.34	1.36	1.27	1.69
% C conversion	39.1	58.9	63.2	50.6	96.8
Dry Make Gas, SCFM	15.6	16.7	16.9	15.6	19.8
Sweet Gas Heating Value, Btu/SCF	333	349	358	375	407
Mass Balance	101.8	99.3	103.1	99.6	99.1

The Acid Gas Removal System was not used for these runs

TABLE 18 CONTINUED

Gasifier	GO-68B	GO-69B	GO-70	GO-71B	GO-72
Date	11/19/80	12/15/80	1/ 8/81	1/27/81	2/19/81
Avg Bed Temp °F	1787	1720	1781	1798	1797
Pressure psig	105	106	106	105	104
Coal Feed lb/h	63.6	54.8	48.4	45.8	42.3
% Coal	100	100	100	100	100
Steam Feed lb/h	56.8	56.7	57.6	57.3	57.3
S/C Ratio	1.12	1.56	1.81	1.65	1.72
% C Conversion	66.7	68.5	85.9	89.8	82.1
Dry Make Gas, SCFM	23.3	18.9	20.0	21.8	19.5
Sweet Gas Heating Value, Btu/SCF	381	378	379	385	376
Mass Balance	97.9	96.6	95.3	103.5	98.6

AGRS	AMI-43	AMI-44	AMI-45	AMI-47	AMI-52
Date	11/19/80	12/15/80	1/ 8/81	1/27/81	2/19/81
Abs P psig	246	246	447	447	447
Abs Temp °F	-36	.8	-36	-35	-36
Abs Packing ft	7.1	7.1	7.1	7.1	21.3
Liquid Flow gpm	0.7	0.7	1.4	1.4	1.4
Gas Flow SCFM	15.10	14.56	14.13	14.22	14.00
Flash P psig	47	145	147	147	147
Str P psig	9.8	9.9	9.9	9.9	9.9
Str Temp °F	22.1	0.0	-5.6	48	48
Str Packing Ft	21.3	21.3	21.3	21.3	21.3
Str N2 SCFM	1.09	1.09	1.09	1.09	1.09
Mass Balance	103.8	102.3	103.0	104.8	101.4
RTI Analysis	No	Yes	Yes	No	No

TABLE 18 CONTINUED

Gasifier	GO-73B	GO-74	GO-76	GO-78	GO-79
Date	3/12/81	3/25/81	4/28/81	5/20/81	6/10/81
Avg Bed Temp °F	1793	1659	1712	1606	1748
Pressure psig	107	106	101	104	104
Coal Feed lb/h	40.3	67.2	50.9	41.1	36.0
% Coal	100	100	100	100	100
Steam Feed lb/h	57.3	48.6	57.4	57.4	57.4
S/C Ratio	1.90	0.97	1.54	1.72	2.04
% C Conversion	89.4	39.7	74.1	61.6	90.3
Dry Make Gas, SCFM	19.6	15.8	19.2	15.9	18.7
Sweet Gas Heating Value, Btu/SCF	370	377	374	393	366
Mass Balance	97.8	95.3	97.9	98.3	100.6

AGRS	AMI-53		AMI-57	AMI-59	AMI-60
Date	3/12/81		4/28/81	5/20/81	6/10/81
Abs P psig	248	—	447	247	348
Abs Temp °F	-5.4	—	-36	-3.5	-21
Abs Packing ft	7.1	—	7.1	7.1	7.1
Liquid Flow gpm	1.4		0.7	1.4	1.13
Gas Flow SCFM	14.9	—	12.9	12.4	13.3
Flash P psig	144	—	147	144	143
Str P psig	9.9	—	9.9	9.9	9.9
Str Temp °F	48	—	48	48	38
Str Packing ft	21.3	—	21.3	21.3	21.3
Str N2 SCFM	1.09	—	1.09	1.19	1.19
Mass Balance	103.1	—	99.2	101.8	95.5
RTI Analysis	No	—	Yes	Yes	No

MASS BALANCES

The raw data from runs GO-62 through GO-79 were reduced using the data processing program described in Volume II of this report (Ferrell, et al, 1981). Criteria for acceptance of a run defined during operation with the char feed were again used. A run is judged acceptable if the total mass recovery is within 5% of 100%, and if the worst of the recoveries of C, H, and O is within 8%.

The mass balance results are based on the analysis of samples of solid, liquid, and gaseous streams. During operation, care is taken to assure that steady state operation has been achieved before a complete set of samples is taken. This is done by monitoring the reactor temperature and pressure, and the feed and effluent flow rates, and by analyzing the dry make gas approximately every half hour with a Carle gas chromatograph especially set up for this purpose.

The data logging program provides a one page run summary which includes run conditions, total mass and elemental recoveries, carbon conversion, make gas flow rate and heating value, and make gas constituent flow rates. Run summaries for runs GO-62 through GO-79, in both metric and English units, are given in Appendix A.

EFFECTS OF OPERATING PARAMETERS

The reactor temperature and steam-to-carbon feed ratio were the main operating parameters varied in runs GO-66 through GO-79. The reactor pressure was held constant at approximately 790 kPa (100 psig) for all runs, and the inlet gas velocity was approximately 0.33 m/s (1.1 ft/s) for all runs. It was desired to use the same coal feed rate from run to run; however, variations in the efficiency of the screw feed system led to varying coal feed rates.

The effect of the average bed temperature on the dry make gas flow rate is shown in Figure 29. The average bed temperature used here is a volume-weighted average, calculated from thermocouple measurements at four locations within the fluidized bed. For the points shown the molar steam-to-carbon ratio varied from 1.54 to 1.81; this variation is partly responsible for the observed scatter. Figure 30 shows the effect of the average bed temperature on carbon conversion. Figures 29 and 30 show that the make gas flow rate and carbon conversion both increase with increasing temperature. This is to be expected, as the degree of devolatilization and the gasification reaction rates all increase with increasing temperature. The effect of the steam to carbon ratio on reactor performance cannot be clearly shown with the set of runs thus far completed. Although the effects of operating parameters on reactor performance are not easily determined directly from the experimental data, the model to be described in a following section does a reasonably good job of correlating run results.

Previous studies with a char feed (Ferrell et al, 1981) indicated that the sulfur conversion could be roughly estimated by assuming it to equal the carbon conversion. For New Mexico coal, it appears that this crude approximation may also be applicable. Figure 31 plots sulfur conversion vs carbon conversion. The plot, despite some obviously bad points (conversions greater than 100%), indicates that the sulfur and carbon conversions did not differ greatly for most of the runs.

Figure 29
EFFECT OF BED TEMPERATURE ON DRY MAKE GAS FLOW RATE

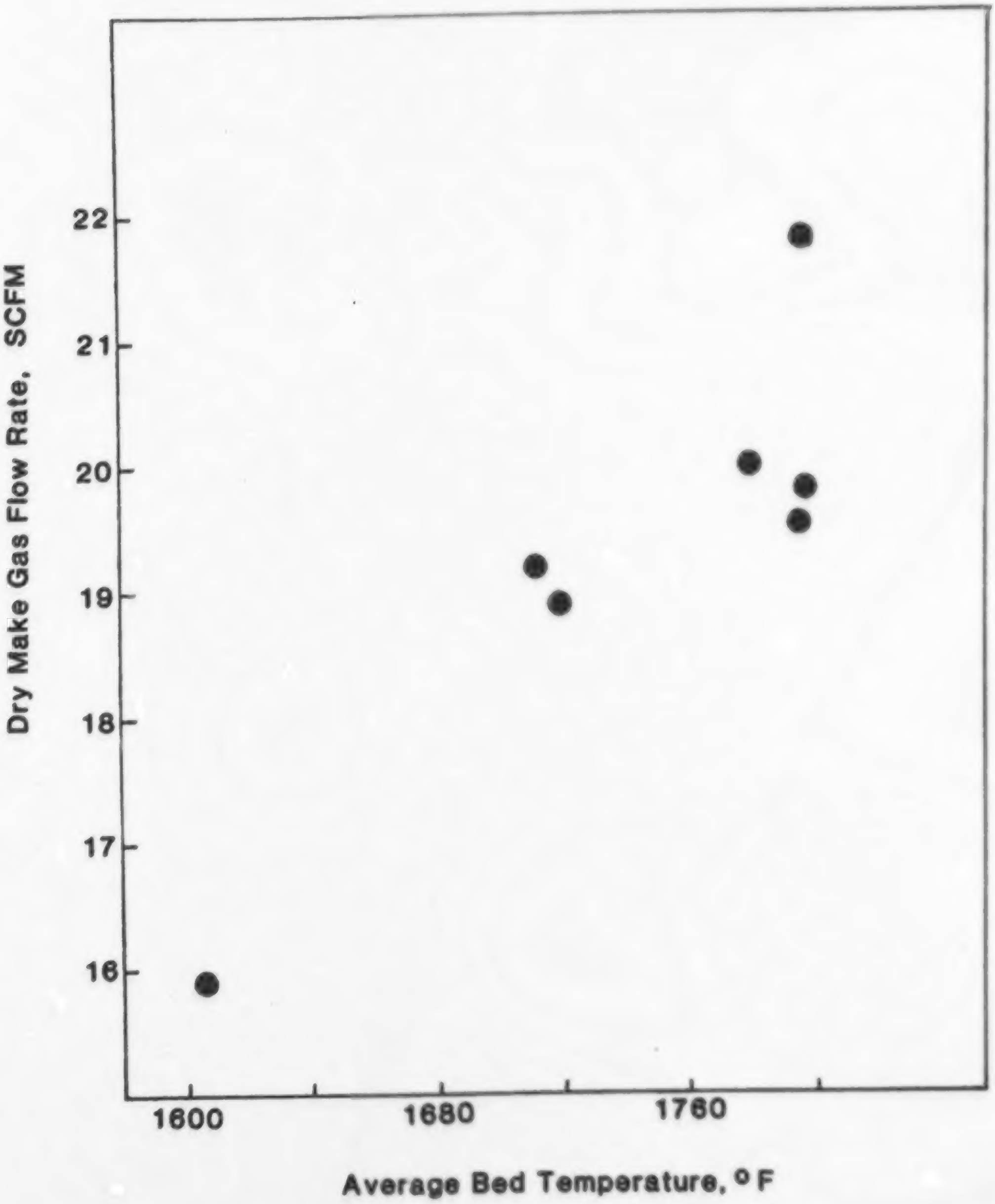


Figure 30

EFFECT OF BED TEMPERATURE ON CARBON CONVERSION

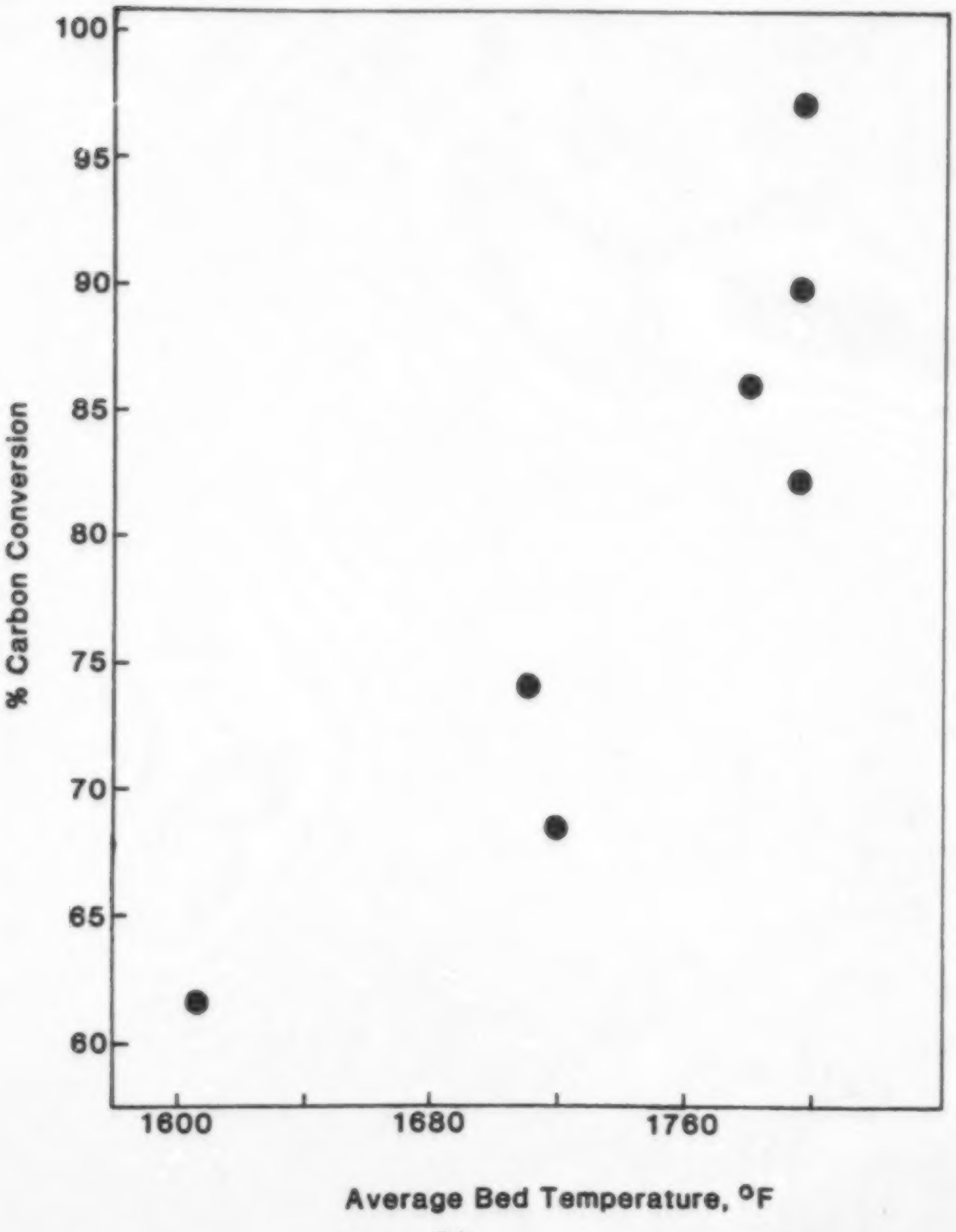
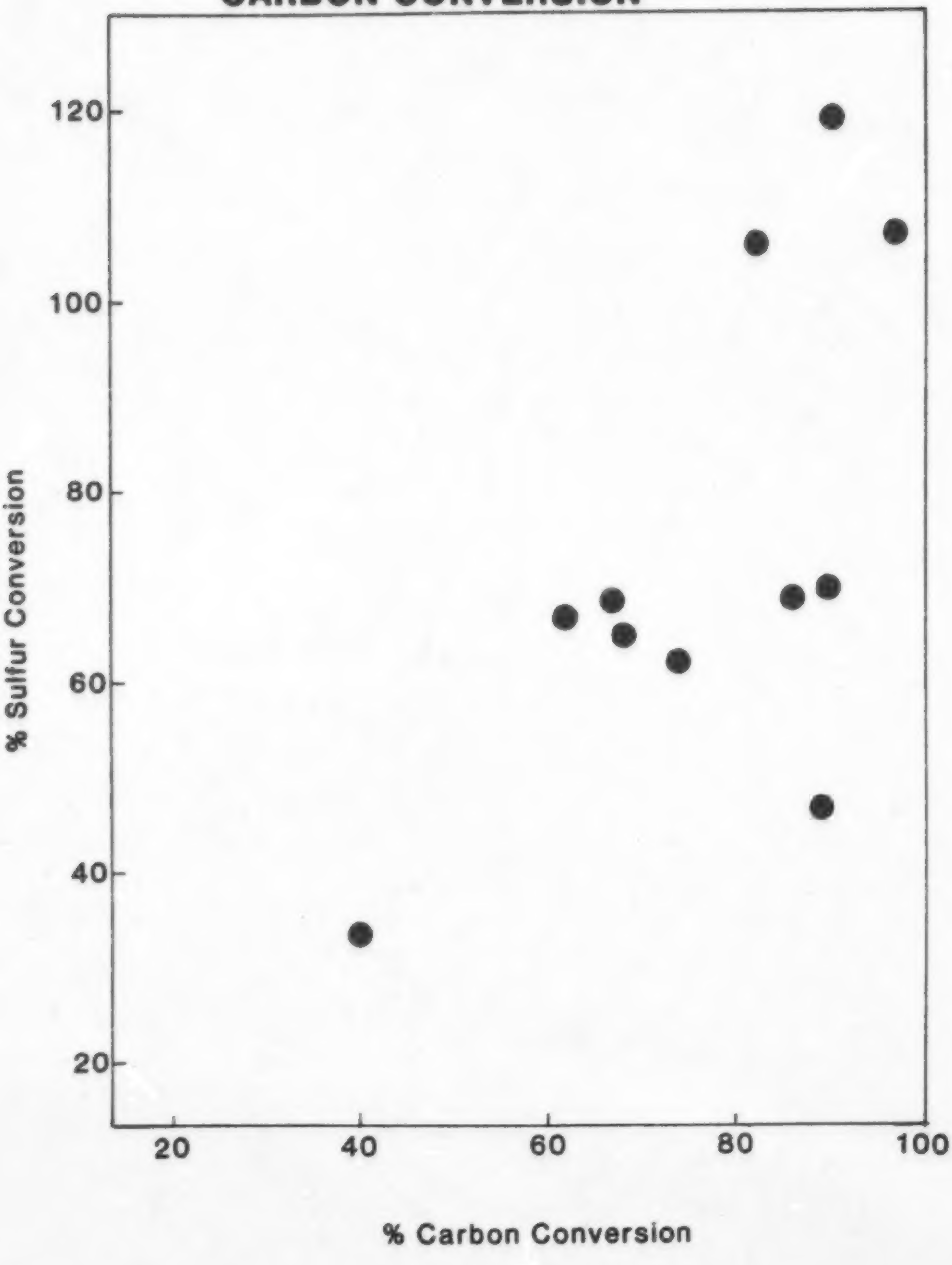


Figure 31
SULFUR CONVERSION VERSUS CARBON CONVERSION



GASIFIER MODELING RESULTS

To aid in the formulation of gasifier performance correlations, a simple model has been developed which considers the gasification process to occur in three stages: instantaneous devolatilization of coal at the top of the fluidized bed, instantaneous combustion of carbon at the bottom of the bed, and steam/carbon gasification and water gas shift reaction in a single perfectly mixed isothermal stage. The model is significant in and of itself, but its particular importance to the project is that it enables the specification of gasifier conditions required to produce a feed to the acid gas removal system with a predetermined flow rate and composition.

In a previous report (Ferrell et al.,1981), the structure of the model was presented, and the ability of the model to correlate data on the gasification of a devolatilized bituminous coal was demonstrated. The model was subsequently extended to include the evolution of volatile gases in the pyrolysis stage of the gasification process, and used to fit the data from the present series of runs with the New Mexico subbituminous coal. The paragraphs that follow outline the revised model, and summarize the data correlations.

GASIFICATION KINETICS

The model takes as input the average reactor bed temperature and pressure, the bed dimensions, feed rates of coal, steam, oxygen, and nitrogen, solids holdup in the bed, and ultimate analysis of the feed coal, and calculates carbon conversion and make gas flow rate and composition.

The model treats gasification as a three-stage process. Devolatilization and combustion are assumed to take place at the top and bottom of the bed, respectively (coal is presumed to be fed at the top, as is done in the pilot plant reactor), and the steam-carbon and water gas shift reactions take place in a single perfectly mixed stage.

Devolatilization is assumed to reach an equilibrium state in the time that the coal falls from the feed screw to the fluidized bed. The equilibrium fractional weight loss, on a dry-ash-free basis, is given by Kau (1980):

$$f_d = 1.052 - 0.7150(T/100) + 0.1615(T/100)^2 - 1.367\times10^{-2}(T/100)^3 + 4.044\times10^{-4}(T/100)^4 \qquad (5)$$

where f_d is the fraction of the dry-ash-free coal devolatilized, and T is the temperature in degrees Kelvin.

The composition of the devolatilization products is taken from preliminary results of devolatilization studies currently being done with a bench-scale batch reactor. The following gas composition is assumed to characterize the dry devolatilized gases: 20% carbon monoxide, 39% hydrogen, 33% methane, 8% carbon dioxide, 0.1% hydrogen sulfide, and 0.02% carbonyl sulfide. Tars are neglected, and it is assumed that water is evolved only by the devolatilization of the moisture fraction of the coal (determined by proximate analysis).

In the fluidized bed, the following six reactions are presumed to take place:

$$C + H_2O = CO + H_2 \qquad (6)$$

$$C + 2H_2 = CH_4 \qquad (7)$$

$$2C + H_2 + H_2O = CO + CH_4 \qquad (8)$$

$$CO + H_2O = CO_2 + H_2 \qquad (9)$$

$$C + 1/2O_2 = CO \qquad (10)$$

$$C + O_2 = CO_2 \qquad (11)$$

Reactions 10 and 11 are the oxidation steps required to supply heat for the remaining reactions. These two reactions are assumed to occur instantaneously in a zone of negligible volume separate from the gasification zone. All oxygen in the feed gas is taken to be consumed to form CO and CO_2, with the combustion product distribution being governed by the relation:

$$C + aO_2 = (2-2a)CO + (2a-1)CO_2 \qquad (12)$$

where a, the combustion product distribution coefficient, is an adjustable model parameter. A value of a = 0.5 indicates that all CO is formed, while a = 1.0 indicates that only CO_2 is formed.

Reactions 6, 7, and 8 are the reactions with which Johnson (1974) at the Institute of Gas Technology correlated gasification kinetics data. Reaction 6 is the conventional steam-carbon reaction. Reaction 8 is assumed to be an independent reaction, although it is attainable as a linear combination of 6 and 7.

The correlation used by Johnson to describe the carbon conversion is given by

$$r = f_L k_T (1-f_c)^{2/3} \exp(-b f_c^{\,2}) \qquad (13)$$

where r is the rate at which the carbon is gasified, k_T is the sum of the rate constants for reactions 6, 7, and 8, f_c is the fractional carbon conversion and b is a kinetic parameter which depends on gas composition and pressure. Expressions for the rate constants and b are given in the previous report (Ferrell et al.,1981). The quantity f_L is given by the expression

$$f_L = f_o \exp(8467/T_o) \qquad (14)$$

where T_o is the maximum temperature to which the coal has been exposed. The reactivity coefficient, f_o, which is an adjustable parameter whose values depend on the particular char used, has values ranging from 0.3 for low-volatile bituminous coal char to about 10 for North Dakota lignite (Johnson, 1974).

Reaction 9 is the water gas shift reaction. The rate expression was given by Wen and Tseng (1979) and reproduced in the previous report (Ferrell et al.,1981), along with an expression for the equilibrium constant K_{IV} as a function of temperature.

REACTOR SIMULATION

The simulation program treats the fluidized bed as three perfectly mixed stages, with devolatilization occurring in the first stage, combustion proceeding to 100% oxygen consumption in the second stage, and gasification taking place in the third.

In the devolatilization stage, the mass of coal devolatilized is determined, and the average molecular weight of the devolatilization gases is calculated. The total and component molar flow rates are calculated, and the coal flow rate and composition are adjusted to account for devolatilization. The devolatilized gases are then assumed to exit from the gasifier, while the devolatilized coal proceeds to the second stage.

In the combustion stage, the molar flow rates of carbon and oxygen are reduced by the appropriate amounts from their feed values, and the flow rates of CO and CO_2 are calculated as

$$q_{CO}' = [2(1-a)/a]q_{O2} \qquad (15)$$

$$q_{CO2}' = [(2a-1)/a]q_{O2} \qquad (16)$$

The effluent from the third stage is next estimated by assuming a carbon conversion of 20% in this stage (based on the carbon flow out of the second stage), with all conversion taking place by the steam-carbon reaction -- eq.(6). The methane effluent rate is estimated to be 1% of the combined molar flow rates of CO, CO_2, H_2, and H_2O. The estimated effluent flow rates along with the reactor temperature and pressure determine the gas composition within the bed (ideal gas behavior is assumed). The component concentrations are then substituted the rate equations to calculate the rates of reactions 6-9.

The calculation of the correct effluent composition from the gasification stage is performed iteratively. In the first iteration, the rates of the first four reactions, $\{r_i^1\}$, calculated as described above, are compared to the following arbitrary values:

$$r_6^0 = 0.01 \qquad (17)$$

$$r_7^0 = -0.0005 \qquad (18)$$

$$r_8^0 = 0.0025 \qquad (19)$$

$$r_9^0 = 0.002 \qquad (20)$$

Rates 6-8 are expressed as fraction of carbon in the bed consumed per minute, while the rate of reaction 9 is in lb-moles/min. Convergence is said to be achieved if the percentage differences between successively determined rates are all less than 0.1%.

Following the calculation of $\{r_i^1\}$, new rates are calculated by modified successive substitution with convergence accelerated by the Dominant Eigenvalue Method (Orbach and Crowe, 1971). For each iteration, the dominant eigenvalue E of the vector of reaction rates is calculated:

$$E^k = \frac{\|\Delta r^{k-1}\|}{\|\Delta r^{k-2}\|} = \frac{\{\sum(r_i^k - r_i^{k-1})^2\}^{0.5}}{\{\sum(r_i^{k-1} - r_i^{k-2})^2\}^{0.5}} \qquad (21)$$

where the superscripts indicate the iteration number. Eigenvalue stability is considered to have been achieved when both of the following conditions are satisfied:

$$\text{(a)} \quad (E^k - E^{k-1})/E^k \leq 0.01 \qquad (22)$$

$$\text{(b)} \quad n \geq 5 \qquad (23)$$

where n is the number of iterations since eigenvalue stability was last achieved. When this condition is met, new rates are calculated as

$$r_i^{k+1} = r_i^{k-1} + p[(r_i^k - r_i^{k-1})/(1-E^k)] \qquad (24)$$

where p is a damping factor.

When eigenvalue stability is not achieved (i.e., when eqs. (22) and (23) are not satisfied), new rates are calculated by modified successive substitution:

$$r_i^{k+1} = qr_{i,c}^k + (1-q)r_{i,e}^k \qquad (25)$$

where $r_{i,c}^k$ is a rate calculated in the k^{th} iteration from the kinetic rate equations, $r_{i,e}^k$ is an estimated rate for the k^{th} iteration, and q is a second damping factor. Preliminary studies showed that damping factor values of p=0.7 and q=0.3 provide rapid and stable convergence; these values were therefore incorporated into the model program.

The new rates are used to calculate new product flow rates for the principal gas components:

$$q_{CO} = q_{CO}' + M_c(r_6+0.5r_8) - r_9 \qquad (26)$$

$$q_{CO2} = q_{CO2}' + r_9 \qquad (27)$$

$$q_{H2} = M_c(r_6-2r_7-0.5r_8) + r_9 \qquad (28)$$

$$q_{H2O} = q_{H2O}' + M_c(-r_6-0.5r_8) - r_9 \qquad (29)$$

$$q_{CH4} = M_c(r_7+0.5r_8) \qquad (30)$$

where M_c is the molar holdup of carbon in the fluidized bed and q_i' is the flow rate of component i leaving the first stage. The flow rates of H_2S and COS are estimated by assuming that the sulfur conversion equals the carbon conversion, and that the following reaction is in equilibrium:

$$COS + H_2O = H_2S + CO_2 \tag{31}$$

The equilibrium constant for the above reaction is defined as

$$K = [CO_2][H_2S]/[H_2O][COS] \tag{32}$$

Values of K are presented by Kohl and Riesenfeld (1979), and are correlated by the equation

$$\ln K = -1.352 + (7881.61)/T \tag{33}$$

where T is in degrees Rankine.

The newly determined product rates are then used in the kinetic rate expressions to calculate reaction rates, and convergence is again checked. This procedure is continued until the convergence criteria are satisfied. After the make gas composition and component flow rates have been determined (by combining the gaseous effluents from the devolatilization and gasification stages), the carbon conversion in the gasifier is calculated as the flow rate of atomic carbon leaving as $CO + CO_2 + CH_4$ divided by the rate at which carbon enters in the feed coal. The make gas flow rate and the fractional steam consumption are also calculated.

MODEL PARAMETER ESTIMATION

In its present form, the model has three adjustable parameters:

1. the coal reactivity coefficient, f_o.
2. the combustion product distribution coefficient, a, which specifies the split between CO and CO_2 in the products of the combustion stage of the gasification.
3. the water gas shift reactivity parameter, f_{wg} .

These parameters were evaluated by using a Pattern Search routine (Beightler et al.,1979) to minimize a function of the sum of squared deviations between predicted and measured values of gasifier performance variables. The function is

$$Y = \sum \left[w_1 \left(\frac{F_p - F_m}{F_m} \right)^2 + w_2 \left(\frac{f_p - f_m}{f_m} \right)^2 + w_3 \left[\left(\frac{y_{H_2,p} - y_{H_2,m}}{y_{H_2,m}} \right)^2 + \left(\frac{y_{CO,p} - y_{CO,m}}{y_{CO,m}} \right)^2 + \left(\frac{y_{CO_2,p} - y_{CO_2,m}}{y_{CO_2,m}} \right)^2 \right] \right] \quad (34)$$

where w_1, w_2, and w_3 are arbitrarily set weighting factors, F is the dry make gas flow rate, f is the total carbon conversion, y_i is the mole fraction of gas i in the product gas, and the subscripts p and m indicate predicted and measured values. The runs with the best mass balance closures (GO-66,68B,69B,71B,72,73B) were chosen to provide the data base for the parameter estimation.

The values of f_o and a were first determined by setting $w_1 = 1$, $w_2 = 1$, and $w_3 = 0$. This weighting scheme was chosen since the predicted make gas flow rate and carbon conversion are highly sensitive to the values of f_o and a, and relatively insensitive to the value of f_{wg}. The results were:

$$f_o = 0.217 \quad (35)$$

$$a = 0.504 \quad (36)$$

With f_o and a being held constant at the above values, the function of eq.(34) was again minimized, with $w_1 = w_2 = 0$ and $w_3 = 1$, in order to determine the optimal value of f_{wg}. This weighting scheme was used as f_{wg} has a large influence on the predicted product gas composition, but only a small effect on the predicted carbon conversion and make gas flow rate. This gave a result of

$$f_{wg} = 3.66 \times 10^{-4} \quad (37)$$

Substitution of the value of a, given above, into eq.(12) indicates that 1% of the carbon oxidized forms CO_2 and 99% forms CO. An equation by Arthur (1951) predicts a = 0.57 at 760°C (1400°F) and a = 0.52 at 1090°C (2000°F), while several gasification studies have assumed a = 1.0 (Caram et al.,1979; Institute of Gas Technology,1978; Pukanic et al.,1978; Sundaresan and Amundson,1979).

The value of $f_{wg} = 3.6 \times 10^{-4}$ indicates that the shift reaction rate is approximately four orders of magnitude less than the rate typically obtained in catalytic shift reactors. Wen and Tseng (1979) used a shift reactivity value of 1.7×10^{-4} in modeling the gasification of a bituminous coal by the SYNTHANE process. The smaller value used by Wen and Tseng may be attributed to the differences between the coals used in both studies.

MODEL PREDICTIONS

Using the optimal parameter values, the model was run for all gasifier runs and a one-page summary is given in Appendix B. Plots of predicted vs measured values of carbon conversion and dry make gas flow rate are shown in Figures 32 and 33. The reasonably close proximity of most points to the 45 degree line is gratifying in view of the simplicity of the model.

The sweet gas heating value was calculated from experimental results and from model predictions for each run. (The sweet gas is defined as the dry make gas with the CO_2 and H_2S removed.) The error between predicted and measured heating values was less than 5% for all runs which satisfied the previously described mass balance criteria.

The model also does a good job of correlating data on the evolution of individual species. Figures 34-36 show predicted versus measured values of rates of emission of H_2, CO, and CO_2 from the gasifier. The good correspondence seen in these plots suggests that the model can be used to predict the composition of the gasifier make gas for a specified set of reactor conditions, and also to study the effects of individual reactor variables on yield.

Figure 37 shows predicted versus measured values of the ratio

$$K = (CO_2)(H_2)/(CO)(H_2O)$$

A high degree of scatter is observed, reflecting the fact that errors in any of the composition variables in K lead to additional errors in the other variable values. In Figure 38, the values of K corresponding to equilibrium at the gasifier exit temperature are plotted against the experimental values of this ratio. The clear tendency of the points to fall above the 45° line, especially relative to the corresponding points on Figure 37, shows the improved correlation that can be obtained by taking the water gas shift reaction kinetics into account rather than assuming equilibrium.

Figure 32

Predicted vs. Experimental Carbon Conversion,
Gasification of New Mexico Coal

Percent

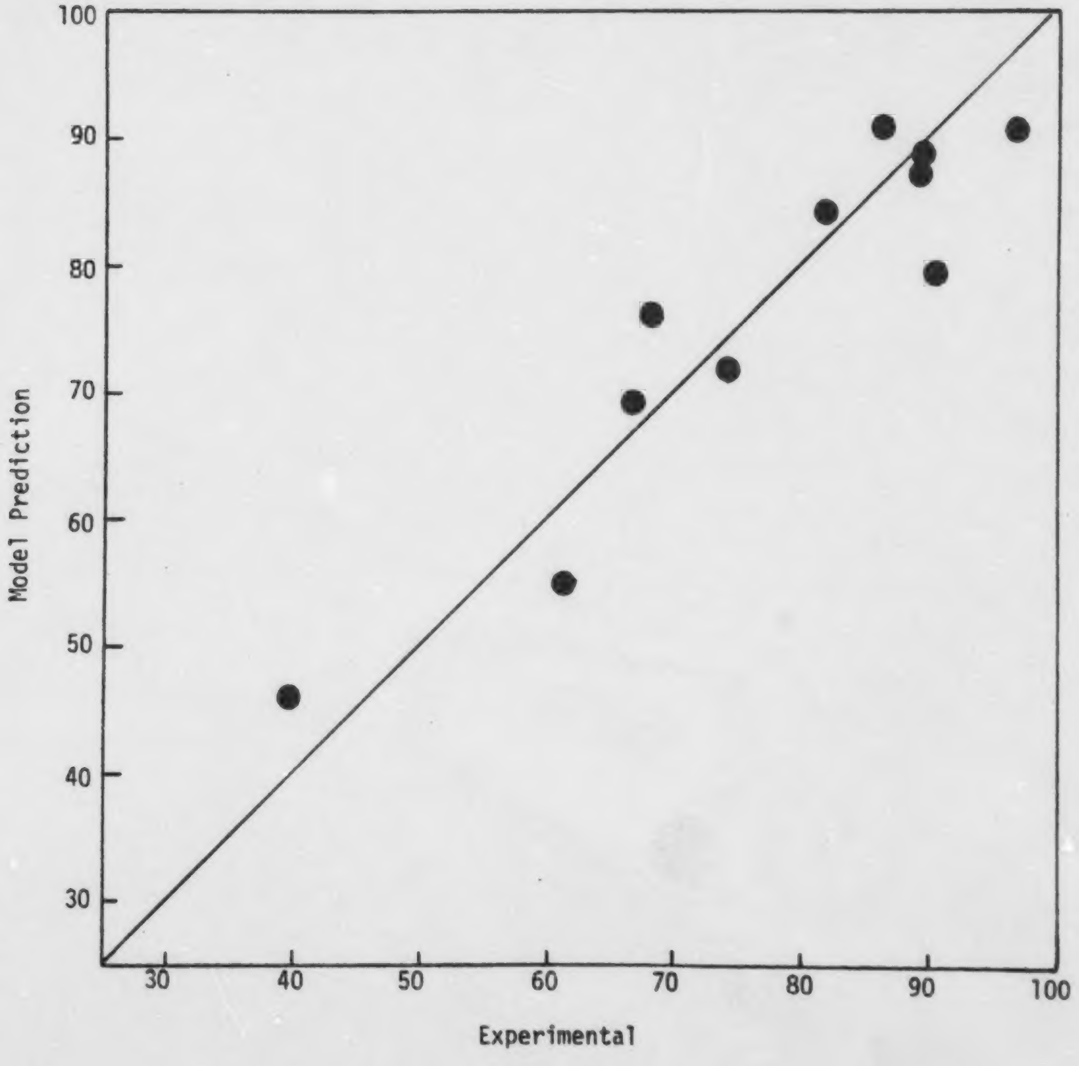


Figure 33

Predicted vs. Experimental Dry Make Gas Flow Rate,
Gasification of New Mexico Coal

SCFM

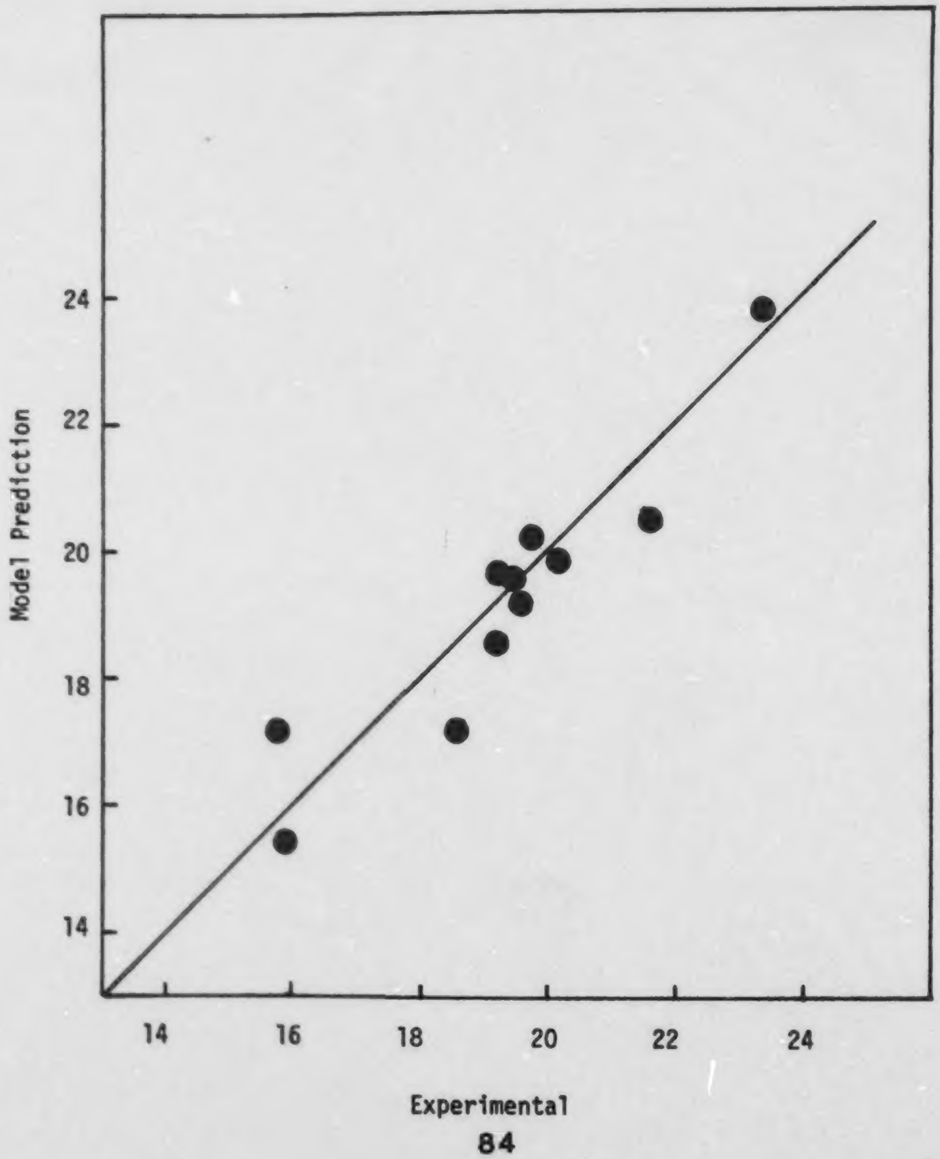


Figure 34

Predicted vs. Experimental
Production Rate of H_2
from Gasification of New Mexico Coal
Lbs/Hr

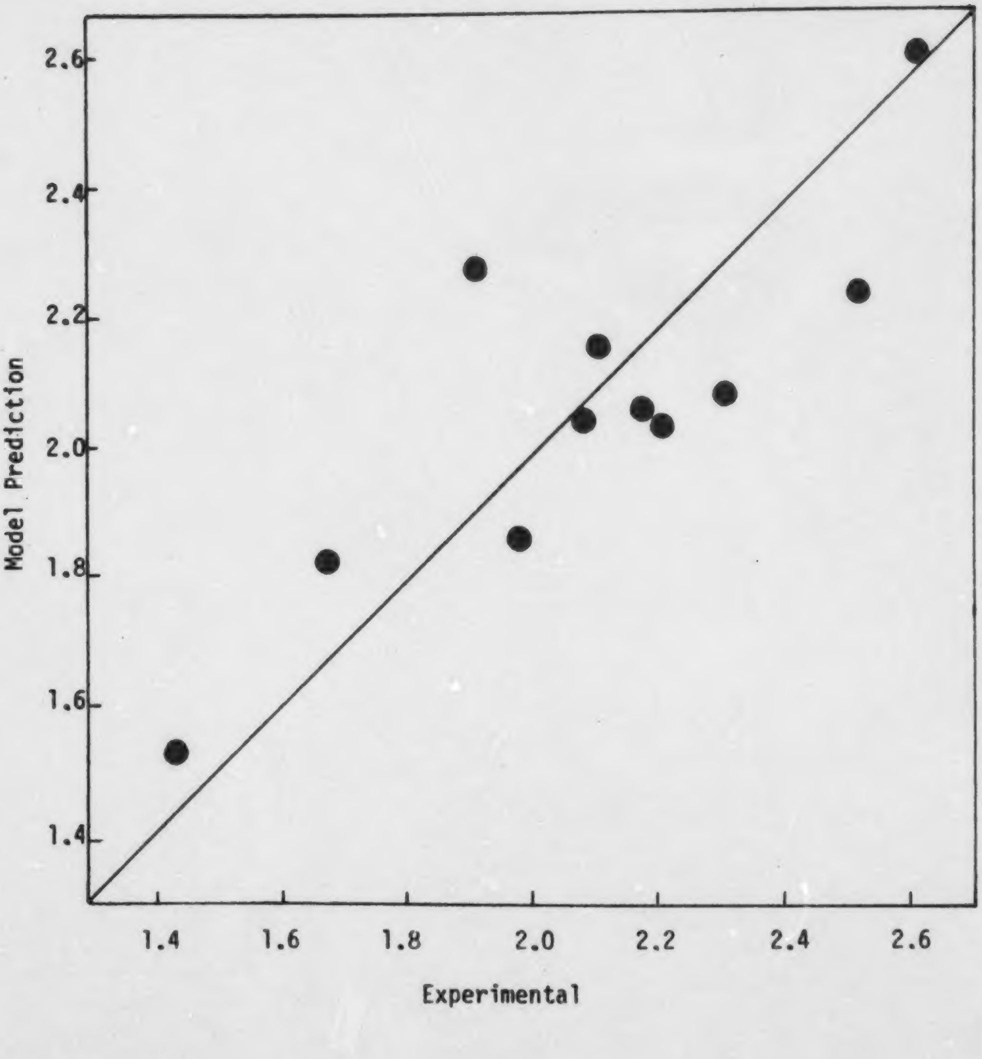


Figure 35

Predicted vs. Experimental
Production Rate of CO from
Gasification of New Mexico Coal
Lbs/Hr

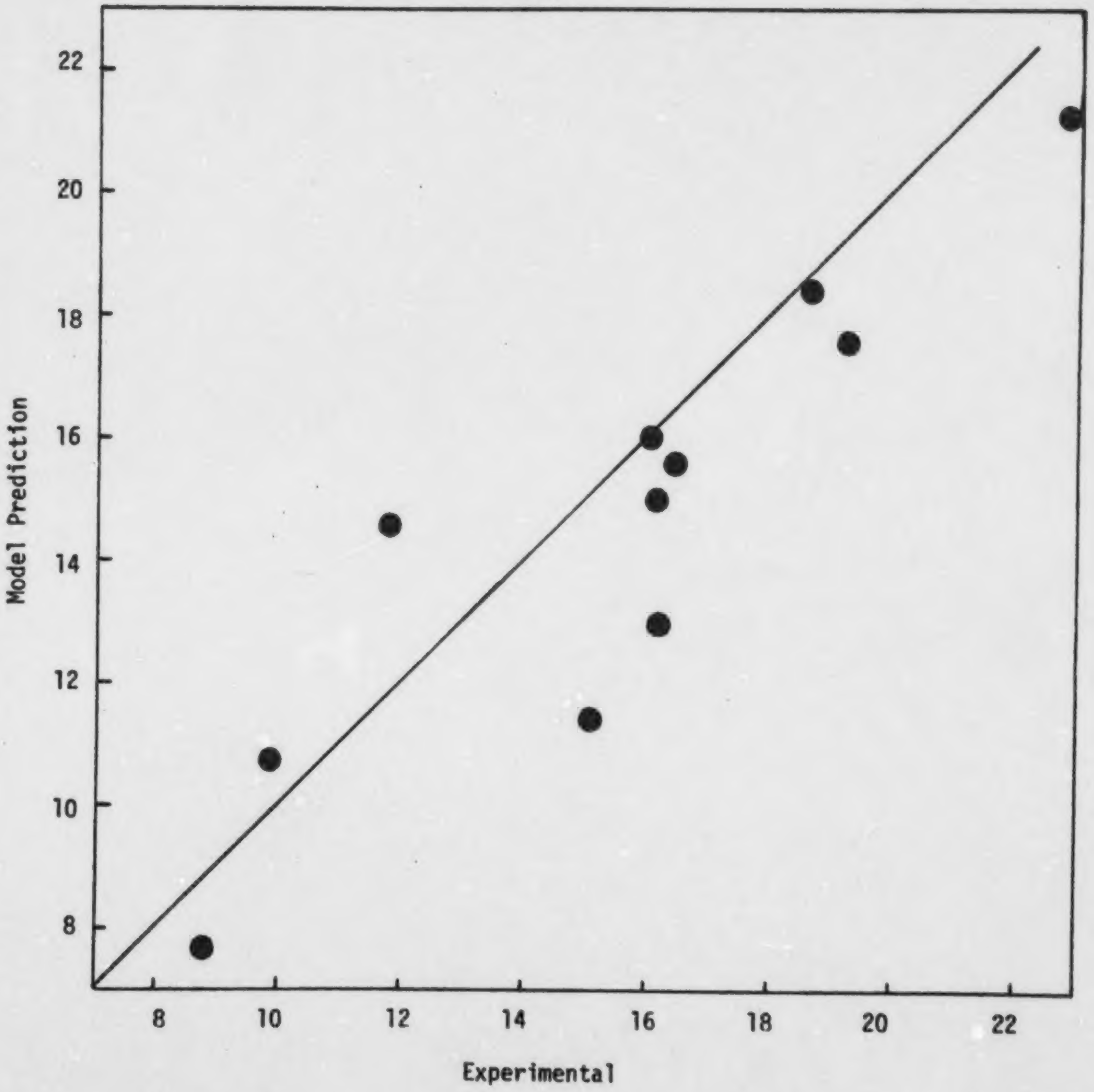


Figure 36

Predicted vs. Experimental
Production Rate of CO_2 from
Gasification of New Mexico Coal

Lbs/Hr

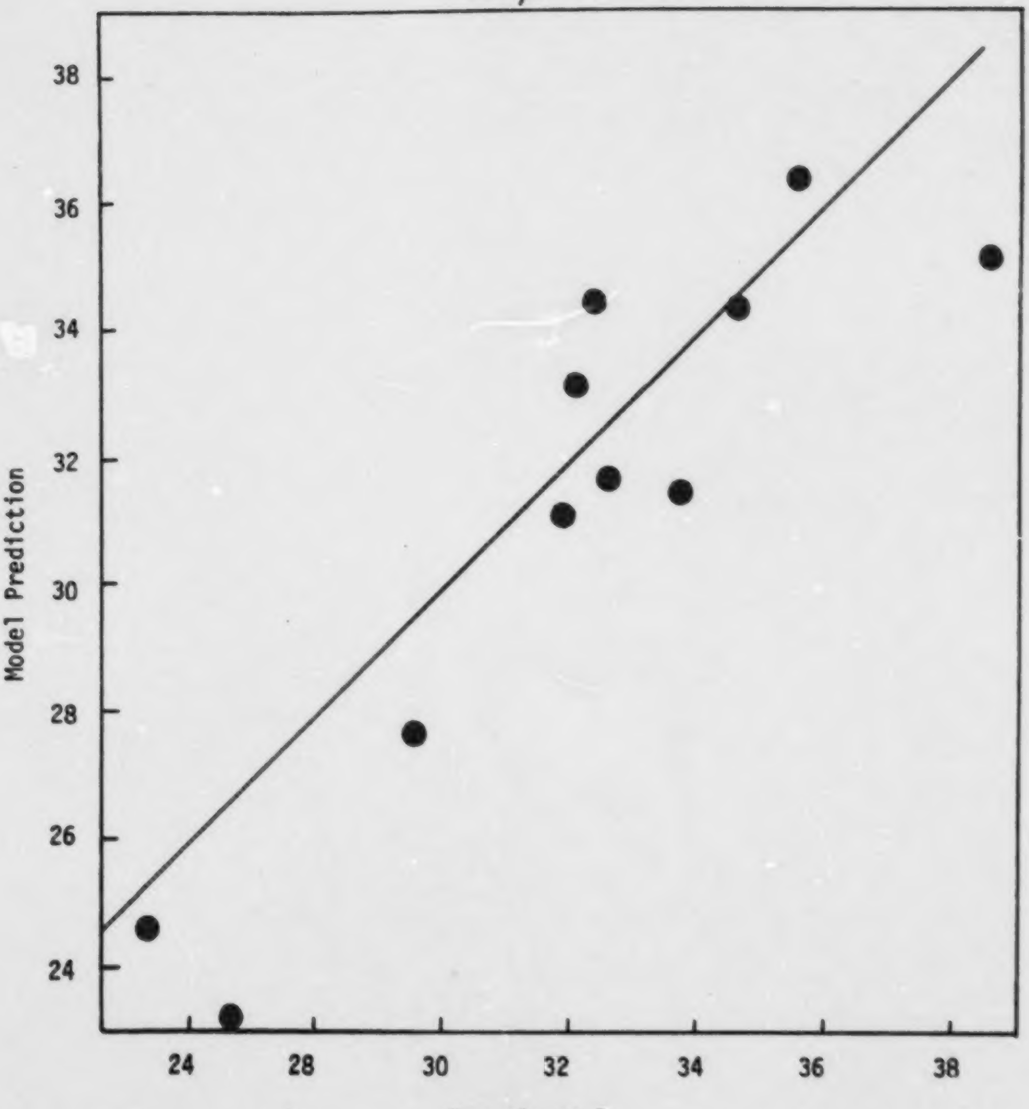


Figure 37

Predicted vs. Experimental K Value,
Gasification of New Mexico Coal

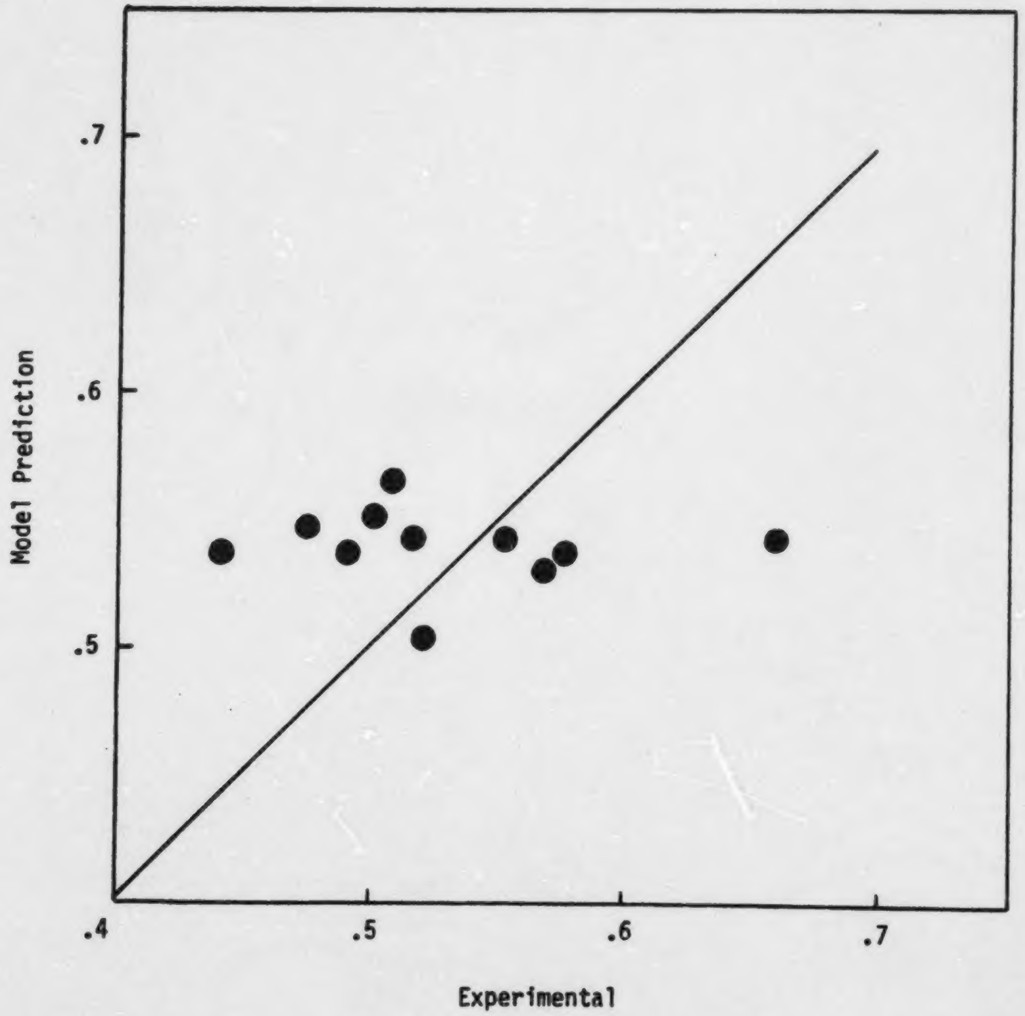
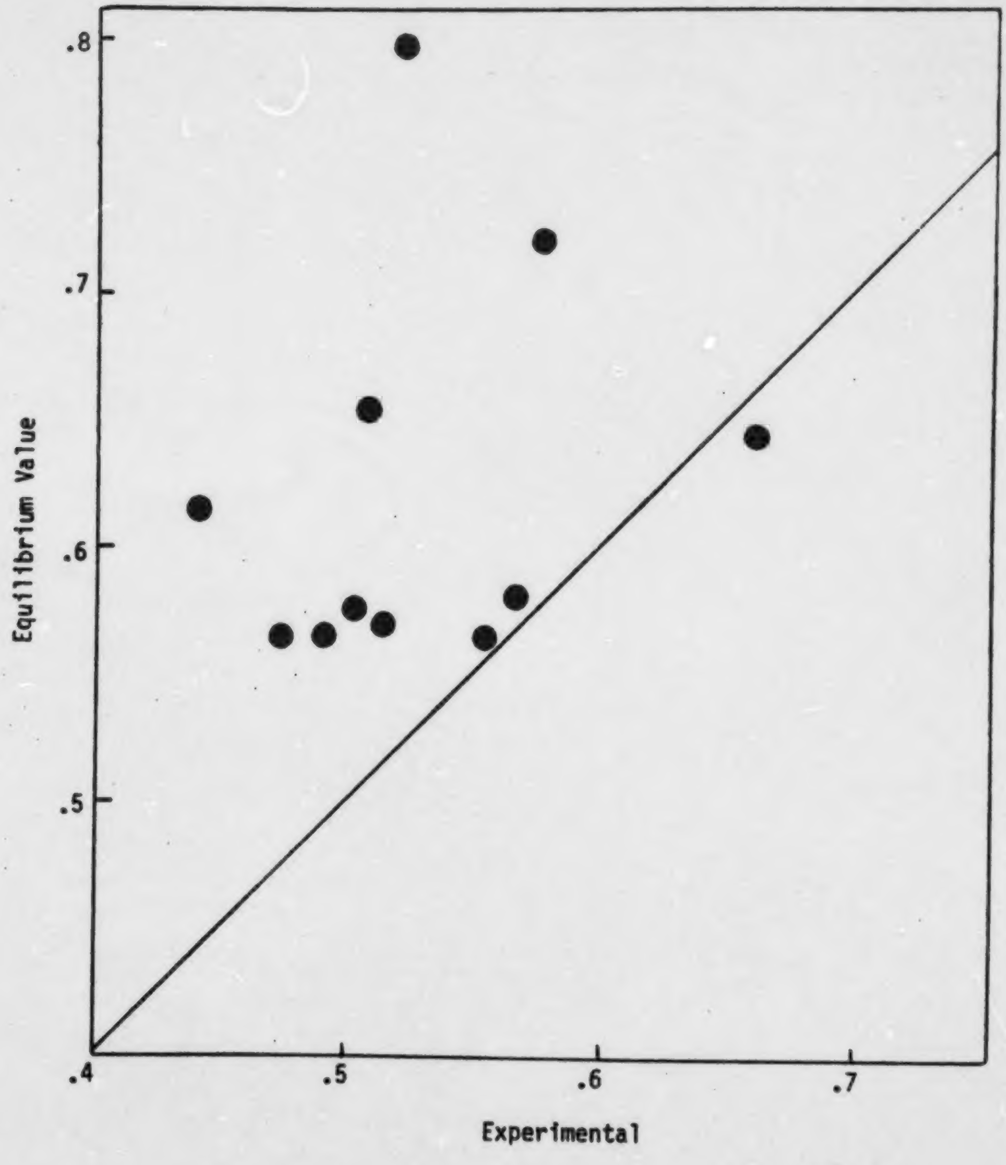


Figure 38

Predicted vs. Experimental K Value
Assuming Equilibrium, Gasification
of New Mexico Coal



EFFECTS OF OPERATING VARIABLES ON REACTOR PERFORMANCE

The model with the optimal parameters determined as described above was run for a number of simulated reactor conditions. Figures 39 and 40 show plots of the effect of gasifier temperature on carbon conversion and make gas production rate for steam-air gasification at fixed steam-to-carbon feed ratios, and Figures 41 and 42 show the effect of steam-to-carbon ratio at fixed temperatures.

Figures 39 and 40, as would be expected, indicate that carbon conversion and make gas flow rate both increase sharply with increasing temperature. The plots also indicate that at low temperatures the steam-to-carbon ratio has little effect on carbon conversion and dry make gas rate.

Figures 41 and 42 show that an increased steam to carbon ratio tends to increase the carbon conversion and make gas production. This is due to the increased rate of the steam-carbon reaction, which increases with increased steam partial pressure. The effect is most dramatic at high temperatures.

FUTURE MODELING STUDIES

Improved hydrodynamic fluidization models are currently being developed, one of which will be incorporated into the gasifier model. The principal advantage of the revised model over the present one will be its allowance for axial temperature gradients in the bed, matching the observed profiles in the gasifier. Also, provision will be made for adiabatic reactor calculations, so that the temperature in the reactor for given steam, oxygen, and coal feeds can be predicted rather than being read in as data. Rate laws for sulfur gas evolution kinetics will also be incorporated, eliminating the current method of equating sulfur and carbon conversions.

The pyrolysis studies being carried out in parallel with the gasification experiments will be used to refine the section of the model that deals with this process. In particular, expressions for the rates of evolution of specific hydrocarbon and sulfur gas pollutants will be incorporated into the model. Since it appears that most of these species in the gasifier make gas originate in the pyrolysis stage, a reasonably good correlation of their emissions might be anticipated.

Figure 39

PREDICTED EFFECT OF GASIFIER TEMPERATURE ON CARBON CONVERSION

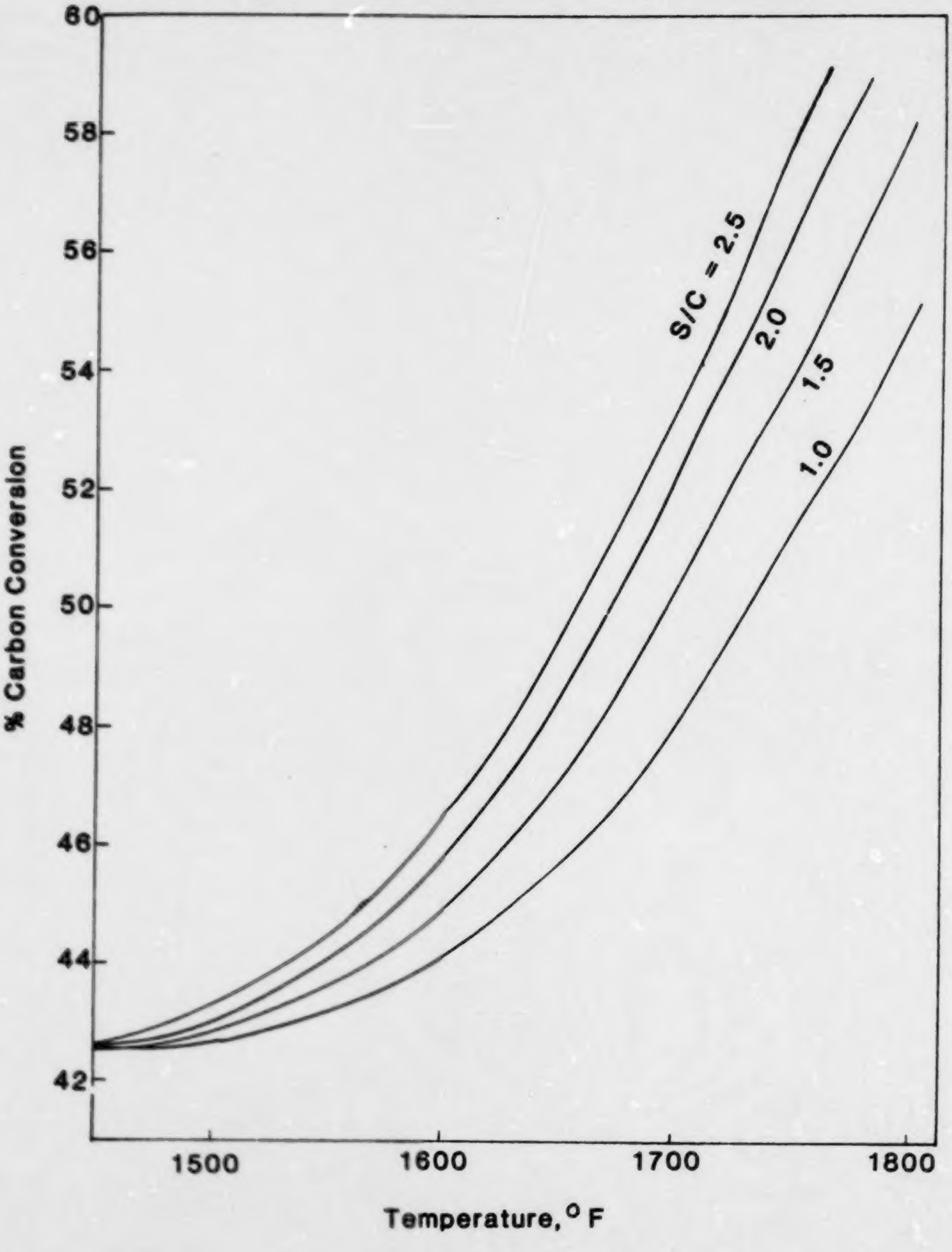


Figure 40

PREDICTED EFFECT OF GASIFIER TEMPERATURE ON DRY MAKE GAS FLOW RATE

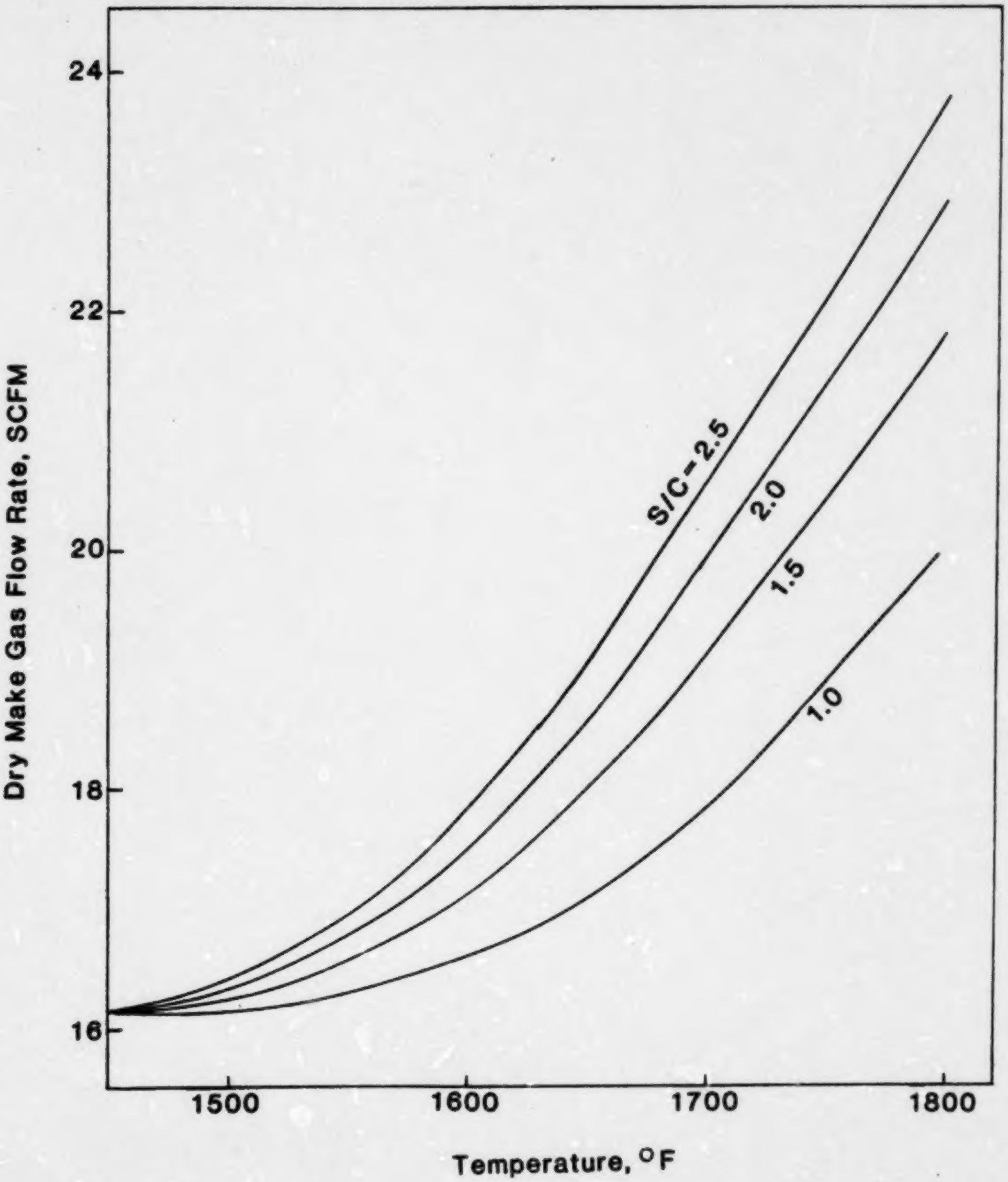


Figure 41

PREDICTED EFFECT OF STEAM TO CARBON RATIO ON CARBON CONVERSION

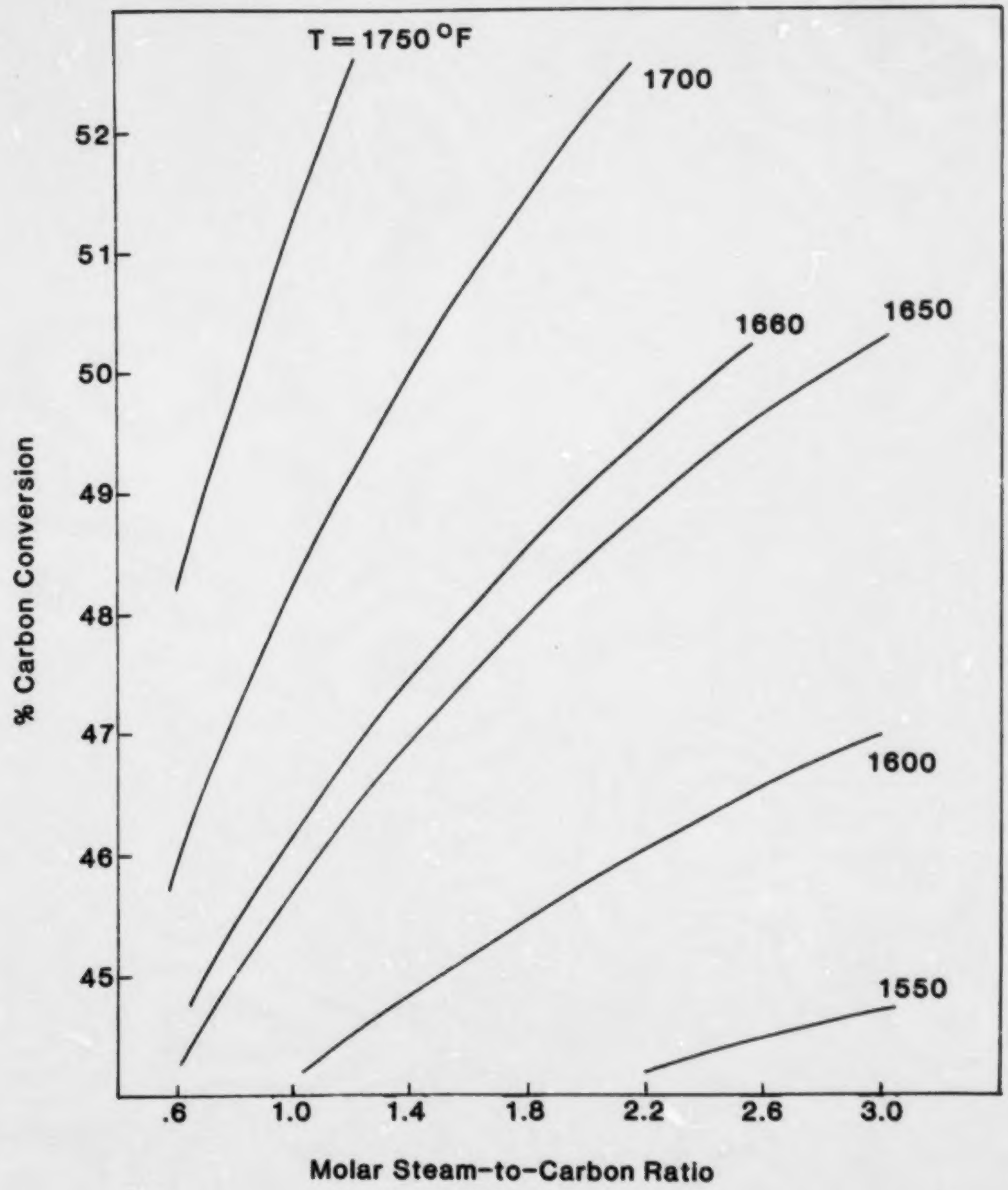
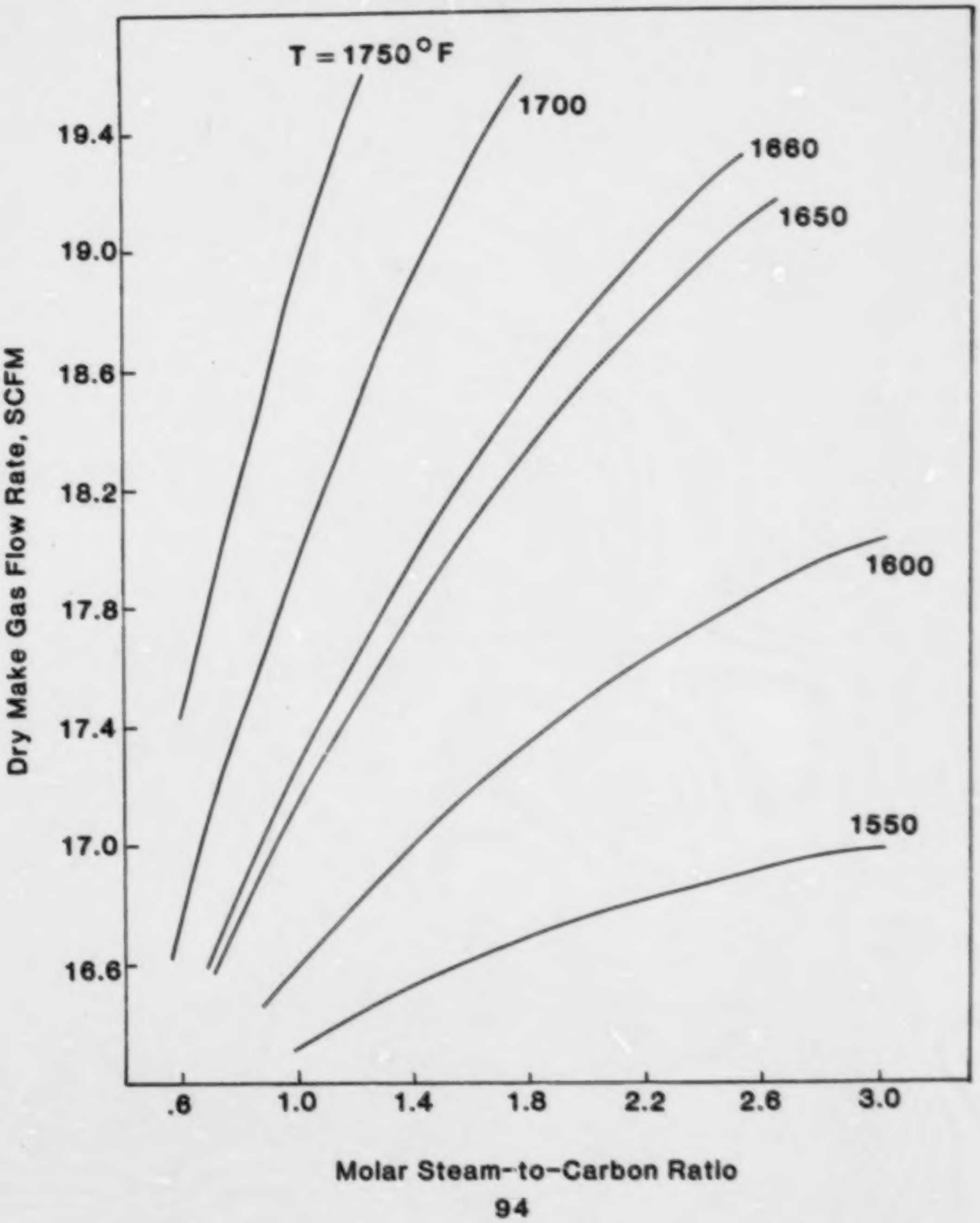


Figure 42

PREDICTED EFFECT OF STEAM TO CARBON RATIO ON DRY MAKE GAS FLOW RATE



ACID GAS REMOVAL SYSTEM RESULTS

A general discussion of acid gas removal systems for coal gasification processes in general, and the Rectisol process using refrigerated methanol in particular, is given by Kelly (1981). This section will present results on emissions from the acid gas removal system.

DESCRIPTION AND OPERATION OF THE ACID GAS REMOVAL SYSTEM

A brief description of the pilot plant system has been given in an earlier section of this report, and a detailed description is given by Ferrell et al. (1980). Several additional features of the AGRS system and its operation will be presented here.

Table 19 presents data on the sizes and operating ranges of the absorber and stripper columns as used in this study.

TABLE 19
COLUMN SPECIFICATIONS AND OPERATING RANGES FOR METHANOL

	ABSORBER	STRIPPER
Total Packed Height	21.3 Feet	21.3 Feet
Column Diameter	5 Inches	6 Inches
No. of Packed Sections	3	3
Packing Type	Ceramic Intalox Saddles	Ceramic Intalox Saddles
Operating Temperature	-35 F TO 0 F	-10 F TO 60 F
Operating Pressure	250-450 psig	10-25 psig
Liquid Flow Rate	0.70-1.40 gpm	0.70-1.40 gpm
Gas Flow Rate	10-20 scfm (at 32 F)	2-10 scfm (at 32 F)

Plant startup began with pressurization of the absorber, flash tank, and stripper with nitrogen from the process nitrogen supply. When all pressures stabilized, the solvent circulation pump was used to move methanol through the system. After the level controllers begin maintaining proper solvent inventory, the refrigeration system was turned on. As soon as some indication of cooling was noted, the sour gas compressor was started and used to pressurize the absorber column to operating pressure, usually between 250 and 450 psig. The flash tank and stripper pressure controllers were set, and the system was ready to accept a feed gas stream from the gasifier-PCS system.

After the feed gas stream entered the bottom of the absorber, a significant amount of heat was released as the acid gas components were dissolved in the methanol. This temperature rise is an indication that the system is operating properly. At this point, all process controllers were in the automatic mode, and the system was allowed to come to a steady state before any samples were taken.

During the startup period of this project, a considerable amount of time was devoted to achieving satisfactory material balance closures. A good material balance depends on stable operation, accurate flow measurement, good sampling techniques and accurate chemical analyses. Second only to sampling, the proper calibration and use of the various flow meters used in the AGRS presented the most difficulty in achieving good mass balances.

The five flow meters used in the AGRS mass balance were all calibrated using nitrogen at a fixed pressure and temperature. For use in the mass balance calculations, the flows indicated by the variable transmitters were corrected by the data acquisition system for the actual pressure and temperature existing at the flow meter. In addition, the mass flow rates must also be corrected for stream composition. This can be done only after chemical analysis, and is a part of the data reduction- mass balance program. Frequent calibration checks were made during the course of this experimental program. A detailed discussion of flow meter calibration and correction is given by Kelly (1981).

Complete mass balances for all runs are given in Appendix E.

RESULTS

The purpose of this study was to evaluate the environmental consequences of the use of methanol as an acid gas removal solvent in coal gasification systems. Although the Rectisol process, which uses refrigerated methanol, has been used by Lurgi since the early 1950's, little is known about the fate of several environmentally significant compounds after they have entered the gas cleaning unit. Under carefully controlled conditions, measurements were made to determine how these compounds distribute through the acid gas removal system for different process situations.

The results from the integrated runs which were made to evaluate methanol as an acid gas removal solvent can be divided into two sections. The first section consisted of four runs made with make gas produced by the gasification of a Western Kentucky bituminous coal char that had been coked at 2000°F. These runs have been discussed in detail in Volume II of this report series (Ferrell et al., 1981), and are included in Appendix E for comparison. The second section consisted of nine runs made with a make gas produced by the steam-oxygen gasification of a New Mexico subbituminous coal obtained from the Navaho mine of the Utah International Coal Company in New Mexico. The difference between these two feedstocks is reflected in the composition of the gas fed to the acid gas removal system.

As previously mentioned, the coal was fed into the fluidized bed gasifier by a top feeding arrangement. The coal, which had been ground to 10 x 80 mesh, was allowed to fall freely from the top of the gasifier into the fluidized bed through zones of increasing temperature where a substantial amount of devolatilization occured. The large amount of tars and oils produced during this devolatilization step necessitated some system redesign because of line blockage in different parts of the particulate removal and gas quenching sections.

While most commercial fluidized bed gasifiers will use a deep-bed injection method of feeding coal into the fluidized bed, it was decided not to modify this system for the runs discussed here. Deep bed injection of coal particles into a fluidized bed minimizes tar and oil production by avoiding devolatilization of the coal during free-fall into the reactor. By injecting coal into a hot fluidized bed, many of the tars and oils formed are cracked into lower molecular weight compounds, thereby minimizing many downstream processing problems. However, since the objective of this study was to evaluate the environmental consequences of using methanol as the acid gas removal solvent, it was thought that the composition of the gas stream fed to the AGRS should be similar in composition to that found in the Lurgi process where methanol is used for gas cleaning. The Lurgi process, in which a fixed bed reactor is used to gasify coal, typically operates at a lower temperature than fluidized bed processes, and produces relatively large quantities of tars and oils.

In addition to the coal feeding method, it should be noted that the relatively simple acid gas removal system used in this study lacks the complexity of the selective systems found in many of the more recently developed physical absorption processes. These later systems, which use more than one absorber and stripper, and often several flash tanks, separate sulfur gases from carbon dioxide before further processing of the acid gas. This is done to concentrate the sulfur gases before they are fed to a sulfur recovery unit, and to recover the CO_2 or vent the CO_2-rich stream to the atmosphere. However, rather than modify the simple system to be physically more representative of a specific selective process, it was believed that data obtained from a single well-characterized system would be of more use than data obtained from a fairly complex system that was similar but not identical to any existing commercial system. Through judicious use of process simulation and engineering calculations, data obtained from this relatively simple pilot plant system can be extrapolated to more industrially-significant situations. In the future, as specific problem areas are identified, the pilot plant will be operated in such a way as to maximize the understanding of these problem areas.

Experimental Program

In designing the experimental program to be used in the coal gasification studies, several approaches were considered. Much of the earlier work with char gasification had shown that reproducibility in gasifier performance was adequate but variability from run to run had to be expected. Also, as was noted during Syngas runs, relatively large changes in process conditions in the AGRS had, in many cases, a minor effect on system performance. The use of a full factorial experimental design was deemed inappropriate for these reasons.

With these factors in mind, the experimental program was designed to cover the broadest range of operating conditions possible for this system of New Mexico coal and refrigerated methanol. The effect of systematically varying important process variables on system performance was examined by comparing all runs to a base case. Although this approach is not exhaustive, it does provide a framework with which to examine the environmental consequences of acid gas removal with methanol. In addition, the work done in this study will be useful in developing experimental programs for other coals and acid gas removal solvents to be studied in this facility.

Table 20 shows the operating conditions used for the nine runs made in this part of the study. Run AMI-47 was chosen as the base case with which all other runs were to be compared. Because there were differences in analytical capabilities and resources over the course of these runs, certain trace analyses were not done for some runs. Also, GC/MS analyses of the solvent streams in the AGRS were done only for certain runs.

Presented below is a brief summary of the purpose of each run in the framework of the experimental program. The study here focuses on the operation of the absorber but includes information on the effect of flash tank and stripper operation on overall system performance. Each run is discussed in the following section.

Summary of Run Results

1. AMI-47/GO-71B

This run was chosen as the base case because, with the exception of packing height, it represents the best case for absorber performance. For this run, the absorber liquid flow rate, inlet liquid temperature and column pressure were set to maximize acid gas removal efficiency. Also, the stripper was run at 48°F which was equal to the highest temperature used in this set of runs. This was done to improve stripping efficiency and, thus, absorber performance.

2. AMI-43/68B

This run represents the first successful integrated run with New Mexico coal and refrigerated methanol. A lower absorber pressure and a lower liquid flow rate were used than in AMI-47. Also, the temperature of the solvent fed to the stripper was not controlled and turned out to be 8.4°F. This led to incomplete solvent regeneration and hence a reduced acid gas removal efficiency in the absorber. The flash tank was operated at a lower pressure (4.2 atmospheres) than AMI-47 (11.0 atmospheres) to provide additional information on this part of the process.

3. AMI-44/GO-69B

The objective of this run was to set absorber conditions so that the "worst case" absorber performance would result. In addition, the stripper inlet liquid temperature was not controlled and turned out to be 14.6°F which also hindered absorber effectiveness.

4. AMI-45/GO-70

The conditions for this run were identical to AMI-47 except that the stripper temperature which was set at -5.6°F. This run was used to evaluate the effect of stripper performance on system operation.

5. AMI-52/GO-72

This run was carried out with the same conditions as in AMI-47 with the packing height in the absorber increased from 7.1 to 21.3 feet. This run represented a "best case" for absorber performance.

6. AMI-53/GO-73B

Here, the process variables that influence vapor-liquid phase equilibria were changed in the absorber relative to AMI-47. The absorber pressure was reduced from 31.6 to 18.0 atmospheres and the inlet liquid temperature was increased from -34.9°F to -5.4°F. The objective was to investigate the effect of reduced absorber efficiency on the distribution of various compounds in the AGRS.

7. AMI-53/GO-76

This run was used to determine the effect of liquid flow rate on system performance. All other process variables were kept the same as in AMI-47.

8. AMI-59/GO-78

Gasifier conditions were purposely changed so that a greater amount of hydrocarbon and aromatic species was produced and fed to the AGRS. This was done by operating the gasifier at a lower temperature than in the other runs. AGRS conditions were set as they were in AMI-53. Gasifier operating conditions also resulted in a lower inlet gas flow rate (14.9 SCFM) to the absorber than in AMI-47 (16.8 SCFM).

9. AMI-60/GO-79

This run was made at conditions that were intermediate to those used in other runs. The absorber pressure (21.4 atmospheres), the liquid flow rate (100.8 lb moles/hr/ft^2) and the absorber liquid temperature (-21.0^{o}F) were set between the values used for the other runs. The objective of this run was to provide additional information in constructing a data base in this series of runs.

Discussion

From an environmental perspective, operation of an acid gas removal system in a coal gasification process becomes important when harmful compounds or pollutants are somehow discharged to the atmosphere. Although there are a wide variety of extremely toxic materials released from coal during gasification, as long as they remain within the gas cleaning system or are properly processed, they pose no problem. However, while in most cases, these harmful materials are not purposely discharged to the atmosphere from the acid gas removal system under normal operating conditions, several of the AGRS gas streams are fed to downstream processes. There, inability to handle toxic compounds and pollutants may result in their discharge to the atmosphere. It is, therefore, important to know what compounds enter the AGRS, and how they distribute in the system under various processing conditions.

Summaries of the gas analyses for all runs can be found in Appendix D. Detailed material balance and operating condition reports are included in the Appendices. Gas analysis from six different locations are reported. The sample train sample is taken downstream from the cyclone separator and is the closest sampling point to the gasifier. The unreacted steam in the gas is first condensed and removed before the sample is taken. The PCS tank sample is taken after the gas quenching step but before the dehydrating towers and sour gas compressor. The sour gas sample is taken after the PCS tank and after the gas has been dehydrated, compressed, and cooled to remove the heat of compression. The high levels of several hydrocarbon and sulfur species in the sour gas sample is due to the difficulty of eliminating condensate in the gas sampling lines. A trap located near this sampling station accumulated small amounts of a condensed hydrocarbon phase which was submitted for GC/MS analysis after run AMI-60. It is thought that this sample provides qualitative information on the variety of trace compounds entering the AGRS.

When the system is operating smoothly at steady state, the compositions of the sample train, PCS tank and sour gas samples will be nearly the same. This is some indication of the quality of the run.

Acid Gas Removal--

The primary function of the AGRS is to remove CO_2 and sulfur compounds from the gases produced during coal gasification. Table 20 shows the removal efficiencies of H_2S, COS and CO_2 for the nine coal gasification runs. Using AMI-47 as the base case, the effect of process conditions on acid gas removal can be seen. In run AMI-45, the only difference in operating conditions is that the stripper was operated at -5.6°F rather than at 48°F as in AMI-47. Because the acid gas content of the solvent entering the absorber has a pronounced effect on removal efficiencies, ineffective solvent regeneration in the stripper can be a problem. Comparing AMI-47 and AMI-45, the former shows a significantly better acid gas removal efficiency as a result of the higher operating temperature in the stripper.

The effect of packing height on removal efficiency can be seen by comparing AMI-47 with AMI-52. In AMI-52, 14.2 feet of additional packing was used with only a marginal improvement in the outlet H_2S levels. The acid gas removal efficiencies for the two runs are almost the same.

From these three runs and in examining the results of the other runs in Table 19, it appears that, for the range of conditions studied here, the most significant factor in high acid gas removal efficiencies is stripping efficiency. Even in the case of AMI-44, where a "worst case" set of operating conditions were used, most of the entering acid gases were removed. With the use of more extreme operating conditions and "cleaner" methanol fed to the absorber, the levels of CO_2, COS and H_2S in the sweet gas can probably be reduced to parts per million levels. This is a particularly important point in the case of COS removal which poses problems for many coal gas cleaning systems (Beychok, 1976). If the AGRS solvent can remove COS to sufficiently low levels, the need for catalytically-converting COS to H_2S in an upstream processing step can be avoided (Braun, 1980).

TABLE 20
OPERATING CONDITIONS FOR COAL GASIFICATION RUNS

Run Number AMI-	43	44	45	47	52	53	57	59	60
GO-	68B	69B	70	71B	72	73B	76	78	79
Absorber									
Pressure Atm	18.0	18.0	31.6	31.6	31.6	18.0	31.6	18.0	24.8
Packing Height Ft	7.1	7.1	7.1	7.1	21.3	7.1	7.1	7.1	7.1
Inlet Liquid Flow	63.6	63.5	129.3	130.5	127.9	127.5	61.7	127.3	100.8
Inlet Solvent Temp	-36.1	0.8	-36.3	-34.9	-35.7	-5.4	-36.2	-3.5	-21.0
Inlet Gas Flow	18.1	17.0	17.1	16.8	16.8	17.9	15.4	14.9	16.0
Inlet Gas Temp F	40.1	47.6	22.3	36.3	38.1	42.5	50.4	44.2	56.4
H_2S in ppm	2950	2900	2550	4682	3023	1710	2868	3180	2139
H_2S out ppm	220	280	260	151	105	172	48	190	260
COS in ppm	119	112	79	133	67	60	76	81	84
COS out ppm	12	10	5	7	6	7	1	4	19
CO_2 in %	20	22	21	22	23	22	22	23	22
CO_2 out %	---	1	3	---	---	---	---	---	---
Flash Tank									
Pressure Atm	4.2	10.9	11.0	11.0	11.0	10.8	11.0	10.8	10.7
Stripper									
Pressure Atm	1.7	1.7	1.7	1.7	1.7	1.7	1.7	1.7	1.7
Packing Height Ft	21.3	21.3	21.3	21.3	21.3	21.3	21.3	21.3	21.3
Stripping N_2 Flow	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3
Inlet Gas Flow	75.0	75.0	75.0	75.0	75.0	75.0	75.0	75.0	75.0
Inlet Solvent Temp F	8.4	14.6	-5.6	48.0	48.0	48.1	48.1	48.1	37.6
Overall Mass Balance Closure									
Gasifier %	98.0	96.6	95.3	103.5	98.6	97.8	97.9	98.3	100.6
AGRS %	103.8	102.3	103.0	104.8	101.4	103.1	99.2	101.8	95.5

All Flows in lb-mole/hr-ft^2

The conversion of COS to H_2S before it enters the acid gas removal system is necessary in many proposed processes for treating coal gases because of the difficulty in removing COS to required levels. Chemical solvent systems often form degradation products with COS and CS_2 while some physical solvent systems cannot be operated at sufficiently low temperatures to remove COS to low enough levels. From the data collected in this study, it appears that refrigerated methanol is effective in removing COS and no unusual solubility characteristics were evident at moderate pressures and low liquid temperatures.

Trace Sulfur Compounds--

There are also several other sulfur compounds present in the gas fed to the AGRS which must be removed. Inspection of the tables in Appendix D shows the distribution of several of these compounds in the AGRS. While there is some scatter in the analyses for methyl mercaptan, thiophene, CS_2, and ethyl mercaptan/dimethyl sulfide, it appears that they were reduced to very low levels in most runs. The appearance in the sweet gas of 17 ppm thiophene in AMI-43 and 31 ppm thiophene in AMI-47 is not clear but is probably the result of sampling problems.

A point of potential environmental significance is that while these compounds are removed to low levels, they are not completely accounted for in the flash and acid gas streams. This can be seen for methyl mercaptan and thiophene which are present in relatively high levels in the feed gas. These compounds will accumulate in the solvent and eventually leave the system in one of three exit streams: sweet gas, flash gas, or acid gas. Because most sulfur recovery systems cannot treat mercaptans and thiophene, they will present emission problems if some additional method of treating these gases is not used. This can be a significant problem because the total sulfur from mercaptans, organic sulfides, CS_2, and thiophene is approximately half of the total sulfur associated with COS. If these compounds appear in the sweet gas, they are likely to affect downstream catalytic processes adversely. The presence of these compounds in the sweet gas stream is also a problem if the gas is to be burned for immediate use because the sulfur in these compounds will be converted to SO_2.

While the distribution of the major acid gases (H_2S, COS, and CO_2) in AGRS can probably be predicted from phase equilibria information and engineering calculations, the low levels of trace compounds in the gas fed to the AGRS make predictive results questionable and experimental data that much more valuable.

Interpretation of results show there to be some pattern of trace sulfur species distribution. The increase in stripper temperature from the low levels of AMI-45 to 48°F for AMI-47 resulted in substantially greater amounts of mercaptan and thiophene in the acid gas stream. The results from AMI-44, which represent the "worst case" for absorber performance, show an increase in mercaptan levels in the sweet gas. Apparently, the conditions used in the absorber for this run were not sufficient to remove the mercaptans to low levels. CS_2 seems to distribute to all exit streams in most of the runs despite the differences in process conditions.

Perhaps the most significant finding here is that over a wide range of processing conditions, the presence of at least small amounts of several different sulfur species is to be expected in all AGRS exit streams and provision must be made for handling the associated problems.

Aliphatic Hydrocarbons--

As the amount of volatile matter present in coal increases, the production of aliphatic, aromatic, and polynuclear aromatic compounds produced during gasification also increases. For the series of runs made here, analytical difficulties prevented measurement of all hydrocarbon species of interest for every run. However, some interesting results were obtained. In the gas phase, the analyis included methane, ethylene, ethane, propylene, propane, butane, benzene, toluene, and xylene. Samples of the methanol leaving the stripper were taken for several runs for GC/MS analysis.

Over the range of conditions studied here, the most significant point to be made about the distribution of aliphatic hydrocarbons is their presence in significant quantities in the flash and acid gases. Although flashing of the methanol down to atmospheric pressure prior to stripping would release most of the hydrocarbons, the CO_2-rich flash gas would still contain substantial amounts of several hydrocarbon species. This stream would require further processing before it could be vented.

In run AMI-57, in which the gasifier was operated at a lower temperature to increase the production of hydrocarbons, the aliphatics (excluding methane) made up almost 4.5% of the acid gas stream and 3.5% of the flash gas stream. While staging the flashing operations may result in a better distribution of these compounds, the total product from the flashing and stripping operations must be either recovered as product, fed to a sulfur recovery unit, or vented to the atmosphere. Since it is unlikely that all of the aliphatic hydrocarbons will appear in the sweet gas, as evidenced by the data collected here, additional treatment will be necessary to prevent their eventual appearance in a vent stream.

As was the case with the trace sulfur compounds, there appears to be no unusual pattern of distribution of aliphatic hydrocarbons in the AGRS. The lighter hydrocarbons, methane, ethylene, and ethane, seem to distribute as would be expected from a Henry's law relationship. Their solubilities, though, are probably greater than would be expected from Henry's law information, especially at the high pressures used in the absorber. This is evident from the lower than predicted levels of ethane and ethylene in the sweet gas in several of the runs.

The heavier aliphatics, propylene, propane, and butane, are absorbed to a greater extent than ethane and ethylene. They distribute between the flash and acid gas streams or accumulate in the recirculating solvent. For several runs in which higher stripping temperatures were used, the heavier aliphatics comprised more than 0.5% of the acid gas stream. If the flashing process does not remove most of these compounds prior to stripping, they will end up in the CO_2-rich vent stream and present a significant environmental problem.

Aromatic Hydrocarbons--

Because of the large amount of aromatic hydrocarbons produced during coal gasification, the potential for environmental problems is great. These compounds, which range from benzene to polynuclear species of many forms, must be prevented from escaping from the gas cleaning process for obvious reasons. Their distribution throughout the gas cleaning process is, therefore, of great concern.

The simpler aromatics, benzene, toluene, and xylene, typically make up 0.1% (by volume) of the gas stream entering the AGRS. Of interest is the fact that these compounds tend to accumulate in the recirculating solvent after they have been removed from the entering gas stream. This is evident because the amount of these compounds entering the absorber is not accounted for in the sweet, flash, and acid gas streams.

Analyses performed for selected runs indicate that significant quantities of these compounds are found in the solvent leaving the stripper. Results from three runs are reported in Table 21. These compounds will buildup in the solvent to the point of saturation. If the solvent is not effectively purged of these compounds periodically, they will begin to appear in several different process streams where they will not be properly treated. In this context, emission of these compounds to the atmosphere represents a significant environmental hazard. In larger gas cleaning systems, where heavier hydrocarbons are removed through cold trapping and distilling the stripped methanol, care must still be taken to avoid the emission of these compounds in any CO_2-rich stream that is to be vented. In addition, these compounds must be removed from the acid gas stream sent to the sulfur recovery unit where no provision for treatment exists.

TABLE 21
METHANOL ANALYSIS FOR STRIPPER EXIT
ALL ANALYSES REPORTED IN PPM (VOLUME)

	AMI-44/GO-69B	AMI-57/GO-76
Benzene	190	157
Toluene	200	196
Ethylbenzene	30	87
Xylenes	70	203

Methanol Analysis--

In order to identify the various hydrocarbon species that accumulate in the methanol, samples of the methanol leaving the stripper were taken for several runs. These samples were then analyzed by Gas Chromatography/Mass Spectrometry.

Initial samples taken of the stripped methanol were analyzed by the Research Triangle Institute, Research Triangle Park, North Carolina. The results from AMI-44/GO-69B and AMI-57/GO-76 are shown in Figures 43 and 44 and in Tables 22 and 23. The gasifier conditions for AMI-57/GO-76 were designed to result in the production of larger amounts of heavy organics and tar than the other runs made in this study and this is evident in comparing the spectra from these two runs. The presence of several siloxanes and phthalates are probably related to some contamination of the sample during processing. Results from these runs indicate that most of the compounds accumulating in the methanol are simple aromatics, primarily substituted benzenes. A few C_{10} and C_{11} isomers are identified, indicating that naphthalene is probably present but at trace levels. The presence of trace amounts of C_{14} and C_{15} isomers were found in AMI-57 but they could not be better identified. These may be polynuclear aromatics but they are present in very small amounts relative to the simpler aromatics.

Later in the sampling program, samples from AMI-60/GO-79 were submitted to the GC/MS facility at North Carolina State University for analysis. The results from these analyses are shown in Figures 45 and 46. These Figures show the mass spectra for the stripped methanol before and at the end of the run. Although compound identification was not performed for these analyses, comparison of the two spectra do show the relative changes in the levels of hydrocarbons present in the methanol at the beginning and end of the run. This methanol had been used for several previous runs and had accumulated significant quantities of a variety of organic compounds.

TABLE 22

STRIPPER EXIT METHANOL FOR AMI-44/GO-69B

Peak Number from Figure 43	
1.	CO_2
2.	butene isomer
3.	pentene isomer
4.	2-methyl-2-butene
5.	cyclopentadiene
6.	cyclopentene
7.	C_6H_{12} isomer
8.	C_6H_{14} isomer
9.	C_6H_{10} isomer
10.	methyl cyclopentane
11.	methyl cyclopentadiene
12.	benzene
13.	C_7H_{14} isomer
14.	C_7H_{16} isomer
15.	toluene
16.	C_8H_{16} isomer
17.	C_8H_{18} isomer
19.	ethyl benzene
20.	xylene (M,P)
21.	styrene
22.	xylene (0)
23.	C_9H_{18} isomer
24.	C_9H_20 isomer
25.	$C_{10}H_{20}$ isomer
26.	$C_{10}H_{22}$ isomer
27.	$C_{10}H_{22}$ isomer
28.	------------
29.	$C_{11}H_{24}$
30.	methyl undecane
31.	$C_{11}H_{24}$ isomer
32.	Sat'd hydrocarbon
33.	phthalate
34.	Sat'd hydrocarbon

FIGURE 43
ANALYSIS OF STRIPPER EXIT METHANOL
FROM AMI-44/GO-69B

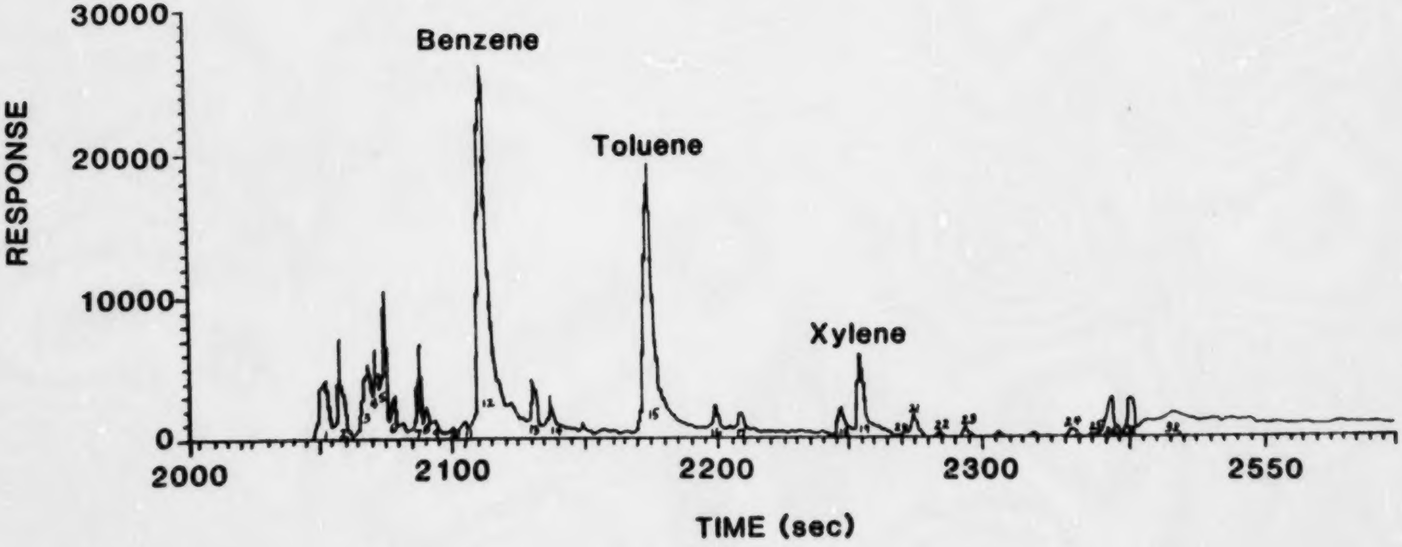


FIGURE 44

RUN NUMBER AMI-57/GO-76
RTI ANALYSIS OF METHANOL AT STRIPPER EXIT
GC/MASS SPEC

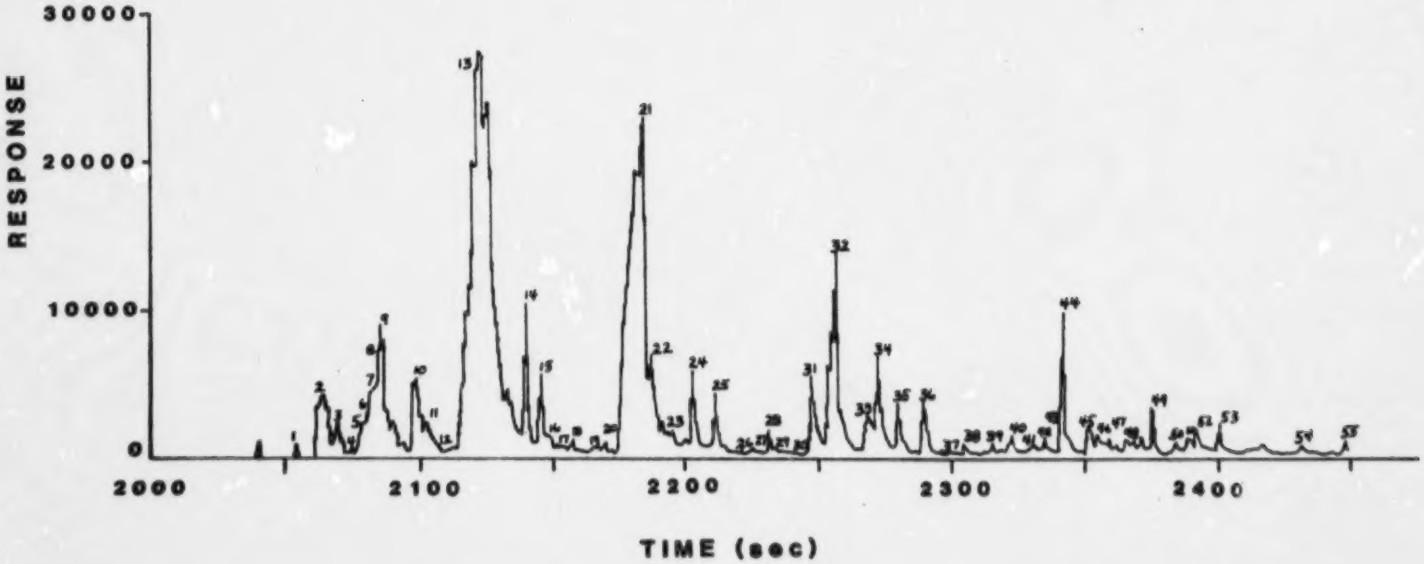


TABLE 23
AMI-57/GO-76 STRIPPER EXIT METHANOL

Peak Number from Figure 44

1. sat'd hydrocarbon
2. CO_2
3. C_4H_8 isomer
4. tetramethylsilane
5. trichlorofluromethane
6. C_5H_{10} isomer
7. unknown
8. Freon 113
9. cyclopentadiene
10. C_6H_{12} isomer
11. C_6H_{14} isomer
12. C_6H_{10} isomer
13. benzene
14. C_7H_{14} isomer
15. C_7H_{16} isomer
16. C_7H_{16} isomer
17. C_7H_{12} isomer
18. C_7H_{12} isomer
19. C_7H_{12} isomer
20. unknown hydrocarbon
21. toluene
22. methyl thiophene isomer
23. C_8H_{16} isomer
24. C_8H_{16} isomer
25. C_8H_{16} isomer
26. C_8H_{16} isomer (trace)
27. C_8H_{14} isomer (trace)
28. hexamethyl cyclotrisiloxane
29. C_9H_{20} isomer
30. C_9H_{18} isomer
31. ethyl benzene
32. xylene (M,P)
33. styrene
34. xylene (O)
35. C_9H_{18} isomer
36. C_9H_{20} isomer
37. C_3 alkyl benzene
38. $C_{10}H_{22}$ isomer
39. unknown hydrocarbon
40. unknown hydrocarbon
41. $C_{11}H_{24}$ isomer
42. C_3 alkyl benzene
43. C_3 alkyl benzene
44. $C_{10}H_{22}$ isomer
45. $C_{10}H_{22}$ isomer
46. C_4 alkyl benzene
47. $C_{10}H_{22}$ isomer
48. $C_{10}H_{20}$ isomer
49. unknown hydrocarbon
50. C_9H_{10}
51. C_9H_8 isomer
52. alkyl benzene isomer
53. $C_{11}H_24$ isomer
54. $C_8H_{10}O$ isomer
55. $C_{11}H_{24}$ isomer
56. $C_8H_{10}O$ isomer
57. unknown siloxane
58. unknown siloxane
59. unknown siloxane
60. $C_{14}H_{30}$ isomer
61. $C_{14}H_{30}$ isomer
62. unknown
63. $C_{15}H_{32}$ isomer

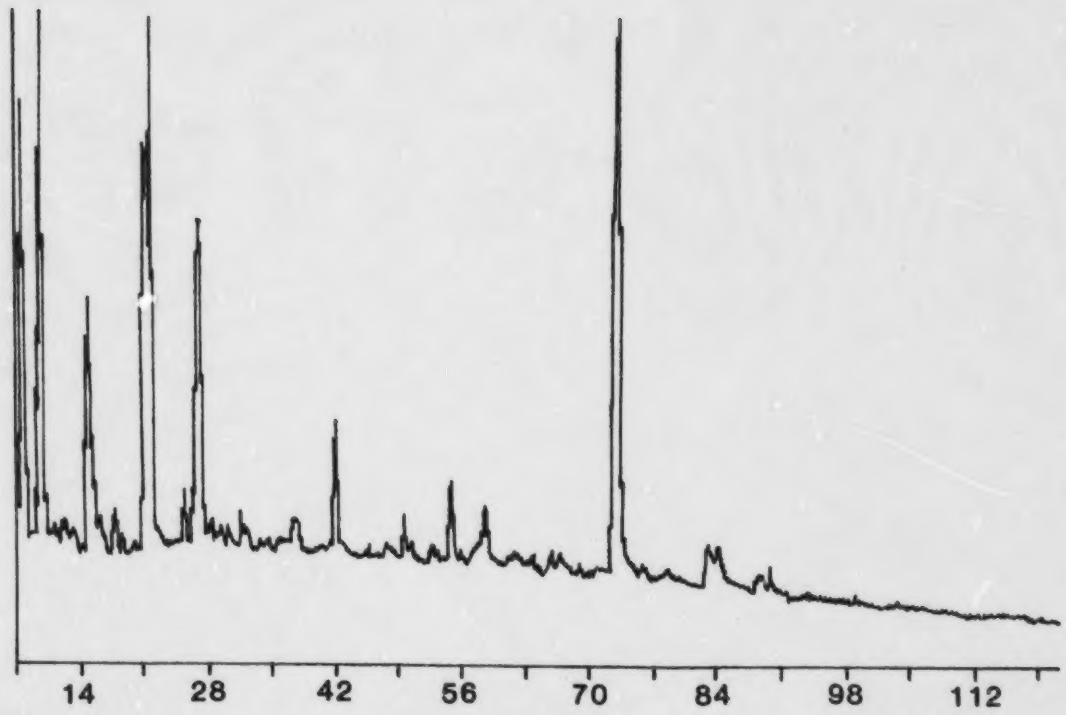


FIGURE 45

STRIPPER EXIT METHANOL BEFORE INTEGRATION FOR AMI-60

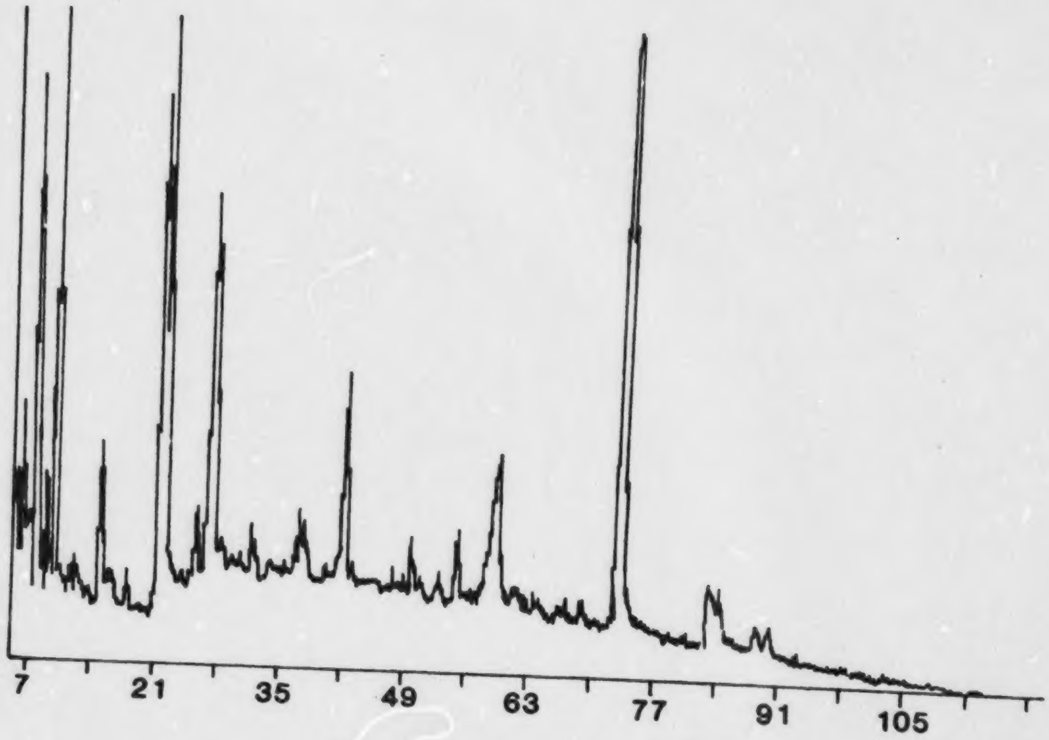


FIGURE 46

STRIPPER EXIT METHANOL TAKEN AT THE END OF AMI-60

The spectra for the sample taken at the end of the run show that the location of most peaks has not changed but the size of several peaks has. This indicates that these hydrocarbons are, in fact, accumulating and will continue to do so until they saturate the solvent. At this point, the presence of these compounds in several process streams is likely and can result in their emission into the atmosphere if proper precautions are not taken.

Samples of liquid condensing in the knockout tank downstream from the sour gas compressor have been discussed earlier in this report and show that the compounds identified were very similar to those found in the stripped methanol from AMI-44 and AMI-57. Again, mostly simple aromatics were found. No polynuclear aromatics were present, which supports the findings of the earlier analyses.

Results from these analyses indicate that very few, if any, polynuclear aromatic compounds were present in the gas fed to the AGRS. This is a particularly important finding. Analyses of the water used to quench the gasifier product gas stream showed that a substantial amount of polynuclear aromatics were present. Evidently, scrubbing of the raw product gas with water effectively removes these compounds allowing only the simpler aromatics to pass through to the AGRS.

Although polynuclear aromatics are removed by the quenching process, substantial amounts of simpler aromatics will be present in the sour gas fed to the AGRS. The use of cold traps may remove some of these compounds but provision must be made to prevent their release to the atmosphere through vent streams or through the sulfur recovery unit. The accumulation of these compounds in the methanol further complicates the problem because of the increased liklihood of their distribution to a number of process streams. The efficiency of solvent regeneration is, therefore, a key factor in avoiding environmental problems.

MODELING OF THE ACID GAS REMOVAL SYSTEM

The evolution and fate of compounds of environmental significance is of primary interest in the operation of the acid gas removal system. In the course of normal operation, several sulfur, nitrogen, and hydrocarbon species are followed as they enter the system and distribute among the three outlet streams (absorber, flash tank, and stripper) or remain in the recirculating solvent. The concentrations of several of these compounds are on the order of a few parts per million by volume, and in order to make any assessment of the effect of process conditions on the distribution of these compounds, steady operation under carefully controlled conditions is necessary. The process modeling summarized here was initiated to provide insight into system performance and to extend experimental findings to process conditions unattainable in the pilot plant.

NON-ISOTHERMAL GAS ABSORPTION IN PACKED COLUMNS

Although a great deal of effort has been expended in the development of calculational techniques for staged absorption columns, much less attention has been focused on packed columns. This is especially true where adiabatic or non-isothermal absorption must be considered. In these cases, the temperature distribution within the column influences solubilities of gas phase components, vapor pressure of the solvent, and values of the transport properties.

Calculational techniques used to describe non-isothermal packed column absorption show varying degrees of complexity. Sherwood, Pigford and Wilke (1975) describe a generalized design procedure for adiabatic absorption in packed towers in which liquid phase resistance to mass and heat transfer and the effect of temperature on transfer coefficients are ignored. von Stockar and Wilke (1977) present both rigorous and short-cut techniques for packed gas absorbers involving large heat effects. A relaxation calculational procedure was used, but only the case of a single transferring solute was described. Rubac, et al (1969) and Bassyoni, et al (1970) use a tray tower analogy to describe non-isothermal gas absorption in packed towers for both simple and multicomponent systems. Only Treybal and Feintuch (1969, 1978) describe an essentially rigorous calculational procedure for the design of a packed absorption column; their procedure includes the influence of thermal effects as well as a capability to handle multicomponent systems. Although they were not able to provide a satisfactory comparison between their model and experimental data for multicomponent systems, it compared favorably for the case of a single transferring solute (Raal and Khurana, 1973).

In this study, an algorithem similar to that of Feintuch and Treybal (1978) was adapted to handle both single solute and multicomponent absorption of acid gases in refrigerated methanol. Adiabatic operation was assumed in the model; this assumption was shown experimentally to correspond to actual system performance. It was also assumed that there was no axial dispersion of either gas or liquid flows. Model predictions and experimental results have compared favorably over a wide range of system operating conditions.

MODEL DEVELOPMENT

In this section of the report, results summarizing the model development will be presented. The model assumes adiabatic operation of the column and uses appropriate mass and energy balances, physical and transport property information, and phase equilibrium relationships to simulate steady-state behavior of the absorber. A subsequent report will present the theory behind the model and document the associated computer programs.

The computer program receives as input the temperature, composition, and flow rates of the inlet gas and liquid streams. The program input also includes column pressure and a specified removal efficiency of the key component (usually CO_2 in the systems studied). Built into the program are physical and transport property subroutines for mixture properties based on techniques suggested by Reid et al. (1977) and Perry (1973). The mass transfer coefficients are determined from the correlations found in Treybal (1980). Heat transfer coefficients are then determined using the j-factor analogy. It was assumed that Henry′s law can be used to express the phase equilibrium relationships for all components. Henry′s law coefficients were taken from Lazalde-Crabtree, et al (1980) or calculated from information found in the literature (Landolt, 1976). Heats of solution at infinite dilution are calculated using the Henry′s law coefficients.

The calculation begins by assuming values for the outlet gas flow rate of each component, including the solvent and the outlet gas temperature. The flow rate of each component in the outlet liquid and the temperature of this stream are calculated from material and energy balances around the column. A stepwise calculation is then begun at the bottom of the column. The calculation then moves up the column by the number of increments specified in the program input until the specified concentration of the key component is reached. At this point, the assumed values of all outlet gas flow rates and the outlet gas temperature is compared to the calculated values. If these values agree within a certain tolerance, the calculation is complete. Otherwise, new values of all outlet gas flow rates and the outlet gas temperature are chosen and the iteration continues.

COMPARISON OF MODEL PREDICTION WITH EXPERIMENTAL RESULTS

To check model predictions against experimental results, calculated liquid temperature profiles are compared to experimental data. In addition, the outlet gas composition and flow rates are compared to measured quantities.

There are two formulations of the model that have been implemented. The first formulation deals with the situation where only one solute is transferred from the gas to the liquid phase. Evaporation and/or condensation of the solvent is also accounted for. This situation is much easier to model than the multicomponent case because the liquid phase consists of only one solute and the solvent; the mole fraction of one component is not independent of that of the other. Also, since the sum of the normalized molar fluxes must be one, the normalized molar flux of the solute is one minus the flux of the solvent; the inert carrier gas does not transfer.

This formulation of the model was tested by comparisons with experimental runs made with the three component system carbon dioxide-methanol-nitrogen. In addition to testing model performance, information concerning the effective interfacial area associated with the column packing was obtained for the mass transfer coefficient correlation used in the model.

As an example of model performance, the operating conditions for AM-32 are shown in Table 24, and a comparison between predicted and experimental liquid temperature profiles in Figure 47. The actual and predicted liquid temperature profiles show excellent agreement in this run where a synthetic gas stream was fed to the absorber from gas bottles.

TABLE 24
PROCESS CONDITIONS FOR SYNTHETIC GAS RUN AM-32

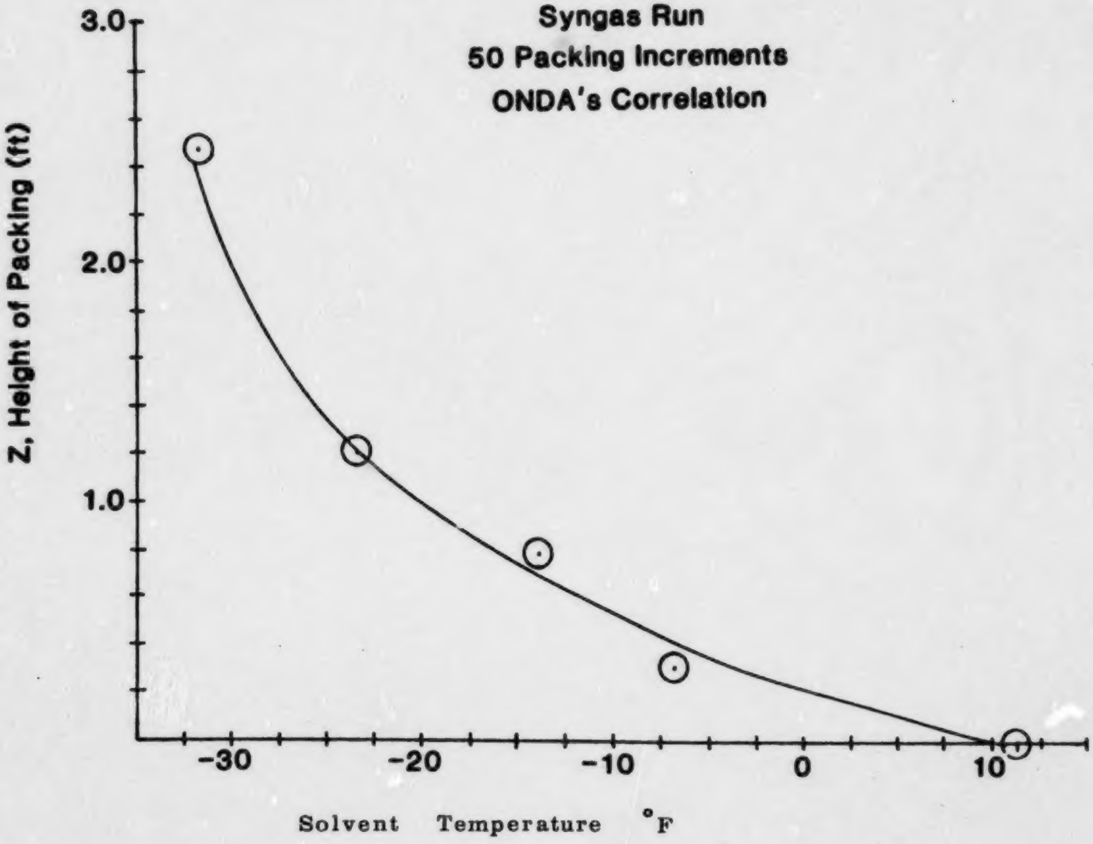
Liquid Flow Rate	61.05 lb moles/hr/ft^2
Absorber Inlet Temperature	-36.1°F
Gas Flow Rate	17.31 lb moles/hr/ft^2
Gas Inlet Temperature	57.4°F
Pressure	28.0 atm absolute
Inlet Gas Composition	33.73 mole percent CO_2 66.27 mole percent N_2
Outlet Gas Composition	0.92 mole percent CO_2 99.08 mole percent N_2
CO_2 Removal Efficiency	98.10%

The other formulation of the model is for mulicomponent cases and is considerably more complex than that described above. This formulation was tested by comparisons with experimental data taken during runs in which the

FIGURE 47

COMPARISON OF MEASURED AND PREDICTED SOLVENT TEMPERATURE

AM-32
Syngas Run
50 Packing Increments
ONDA's Correlation



absorber feed gas was produced in the gasifier. Although there are a wide variety of compounds present in the product gas, the model currently deals with only the nine compounds present in the greatest concentrations. As more data become available, additional compounds will be included in the model.

An example illustrating the comparison between model prediction and experimental data is shown in Tables 25 and 26 and Figure 48. Good agreement is seen between predicted and actual liquid temperature profiles. The difference between the measured temperatures at 4.90 feet have been attributed to electronic problems that were discovered after the run.

TABLE 25
PROCESS CONDITIONS FOR INTEGRATED RUN AMI-43

Liquid Flow Rate	65.10 lb moles/h-ft^2
Liquid Inlet Temperature	-36.13°F
Gas Flow Rate	18.10 lb moles/h-ft^2
Gas Inlet Temperauture	40.13°F
Pressure	17.760 atm absolute

TABLE 26
PREDICTED vs. EXPERIMENTAL RESULTS FOR AMI-43 Compositions in Mole %

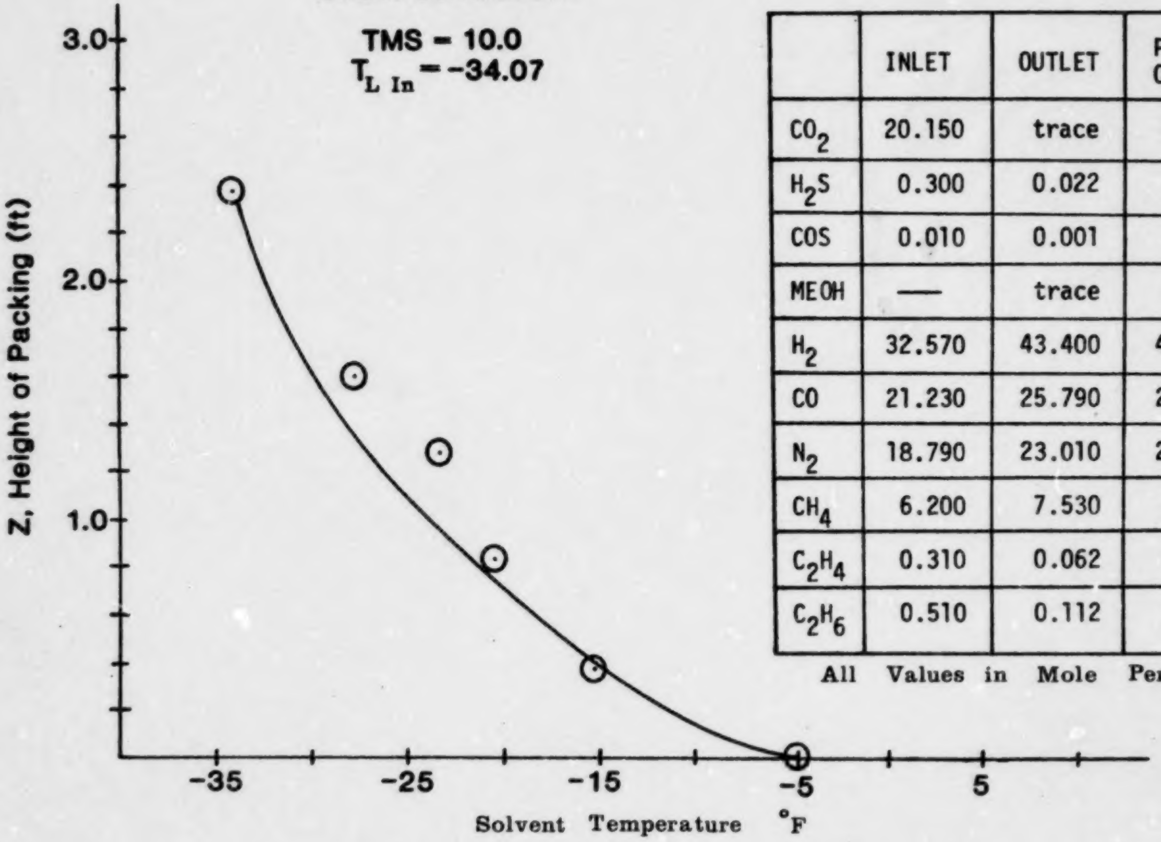
Component	Sour Gas (experimental)	Sweet Gas (experimental)	Sweet Gas (predicted)
CO_2	20.05	trace	0.0128
H_2S	0.295	0.022	<0.0001
COS	0.012	0.001	<0.0001
MEOH	-	trace	<0.0001
H_2	32.42	43.40	41.40
CO	21.23	25.79	26.38
N_2	18.70	23.01	23.50
CH_4	6.59	7.53	8.01
C_2H_4	0.308	0.062	0.218
C_2H_6	0.508	0.112	0.358
Flow rate(SCFM)	15.07	11.81	11.74

While there is very good agreement between the predicted and experimental concentrations for most compounds, as seen in Table 26, data and model predictions for H_2S, C_2H_4, and C_2H_6 do not compare as well as those for other compounds. The difference between experimental and predicted values of H_2S were later shown to be related to the fact that the entering methanol was not adequately stripped and contained some H_2S. The input data to the model assumed that clean methanol was fed to the column. The difference between

FIGURE 48

AMI-43/GO-68B
ONDA Correlation

TMS = 10.0
$T_{L\ In} = -34.07$



	INLET	OUTLET	PREDICTED OUTLET
CO_2	20.150	trace	0.257
H_2S	0.300	0.022	—
COS	0.010	0.001	—
MEOH	—	trace	0.014
H_2	32.570	43.400	41.155
CO	21.230	25.790	26.800
N_2	18.790	23.010	23.748
CH_4	6.200	7.530	7.576
C_2H_4	0.310	0.062	0.163
C_2H_6	0.510	0.112	0.281

All Values in Mole Percent

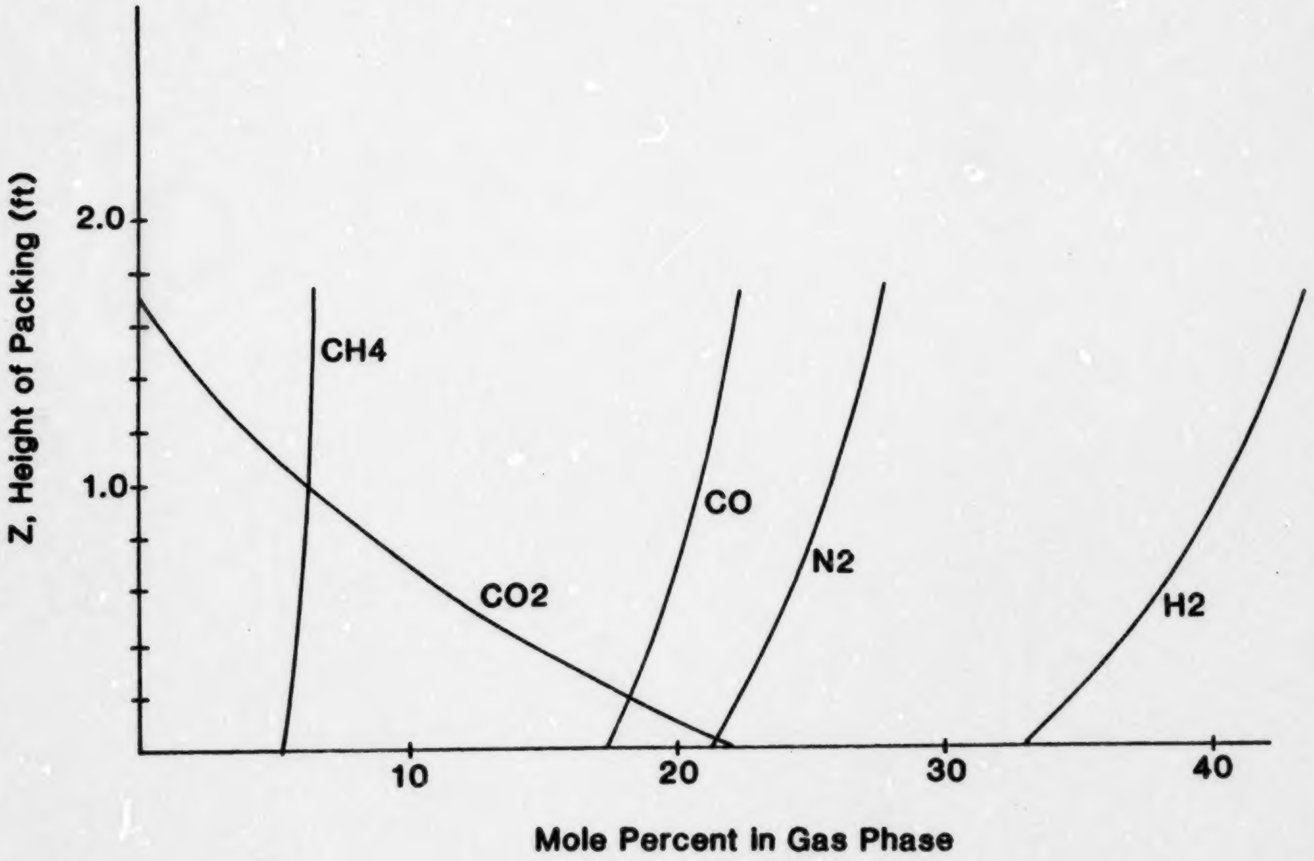
COMPARISON OF MEASURED AND
PREDICTED SOLVENT TEMPERATURE

the values for C_2H_4 and C_2H_6 may be related to the fact that Henry's law is not an accurate assumption for these cases. This point is currently being examined using results from several other runs. Presented in Figure 49 is the computed concentration profiles for all components except COS and methanol which were present in very small concentrations and do not appear on the scale shown. The concentrations of H_2S, C_2H_4, and C_2H_6 are all scaled by a factor of ten.

FIGURE 49

Gas Phase Composition Profile

AMI-53



SUMMARY

A total of 15 gasification runs were made using the pilot plant facility with a New Mexico subbituminous coal. Six runs made use of the gasifier-PCS system only, and nine runs were integrated and included the acid gas removal system.

Gasifier runs were commenced by feeding mixtures of the subbituminous coal and a devolatilized Western Kentucky coal char used in previous studies. This was done in order to evaluate the ability of the system to handle the tars associated with the coal feedstock. Runs GO-62 through GO-65 used 10, 30, 30, and 50 weight percent subbituminous coal, with the balance being char. The success of these runs indicated that 100% New Mexico subbituminous coal could be used as a feedstock, and the remainder of the runs used 100% coal.

Sampling and chemical analysis methods have been developed for all feed and effluent streams. Methods used for the sampling and analysis of gaseous streams are satisfactory for the major gases and for all minor components of the gaseous streams present in concentrations greater than a few parts per million. Detailed chemical compound analyses for solid and liquid streams are generally satisfactory, but are still under development.

A major effort was made to develop methods for the detection of trace metal elements in the feed and effluent streams. Methods used currently for arsenic analysis are satisfactory, both for ease of application and reliability. The principal problem associated with this element is the ineffectiveness of the impinger solutions at trapping it from the gas stream. Reproducibility of lead concentration measurements has been less than satisfactory, although considerable improvement has been made recently by diluting all samples to fall within the linear range of the atomic absorption spectrometer calibration, and by adding dibasic ammonium phosphate to the injected sample, thereby binding the lead and enabling higher charring temperatures. The cold-vapor technique used for mercury is satisfactory; the principal difficulty associated with this element is its volatility, which makes it essential to analyze samples close to the times at which they were taken.

The most important quality assurance test for the evaluation of the experimental data was good closure on the mass balances for total mass and for all major elements. In general, the mass balance results for both the gasifier-PCS system and the acid gas removal system are excellent, and indicate that there are no gross errors in either chemical analyses or mass flow measurements. Frequent calibration checks were necessary to achieve the mass balance results shown.

The reactor temperature and steam-to-carbon feed ratio were the main operating parameters varied in runs GO-66 through GO-79. Results show that the make gas flow rate and the carbon conversion both increase with increasing temperature. This is to be expected, as the degree of devolatilization and the gasification reaction rates all increase with increasing temperature. Although the effects of operating parameters on reactor performance are not easily determined directly from the experimental data, a mathematical model developed in this study does a reasonably good job of correlating run results, and is useful in evaluating the effects of operating parameters.

Previous studies with a char feed indicated that the sulfur conversion could be roughly estimated by assuming it to equal the carbon conversion. For New Mexico coal, it appears that this crude approximation is also applicable. In addition, the results of a detailed analysis of the reactor make gas for the various sulfur gases indicate that the distribution between H_2S and COS may be predicted by assuming that the gases H_2S, COS, CO_2, and H_2O are in equilibrium at the temperature above the fluidized bed.

In the gasification of New Mexico coal a large number of hydrocarbon gases are produced. Aliphatics up to butene and butane and simple aromatic compounds have been detected in the gasifier make gas stream. An analysis of these hydrocarbon emission rates indicates that they generally increase with increasing reactor bed temperature.

After leaving the PCS system, the reactor make gas is compressed to about 525 psig and then cooled to approximately 50^oF. During this process higher molecular weight compounds present in the gas stream in very low concentrations are condensed and separated from the gas in a knockout drum. While a variety of hydrocarbon compounds were found in this liquid, no aromatic compounds heavier than substituted benzenes were found. This fact, together with results of analyses of the methanol AGRS solvent, indicates that no detectable polynuclear aromatic compounds are in the gases leaving the PCS system.

No unusual results were noted from the proximate and ultimate analyses of the solid streams; however, the ultimate analysis of the spent char generally correlates with gasifier run conditions. For example, higher temperatures result in higher carbon conversions and a lower carbon content in the spent char.

The tars collected from the cold trap downstream from the cyclone were subjected to a solvent partitioning scheme in order to separate them into groups of compounds of varying polarities. The groups were then quantified as to their weight percent contribution to the total tar composition. In addition to the partitioning analysis, the tars were analyzed for polynuclear aromatic hydrocarbons and organic sulfur compounds. The PNA's were analyzed by glass capillary gas chromatography with a flame ionization detector, and the sulfur-containing species were analyzed by gas chromatography with a flame photometric detector.

The analyses of the tars indicate that a significant amount of PNA's are in the gas stream as it leaves the reactor, and emerge primarily in the stream condensed by the venturi scrubber. It appears that compounds with boiling points higher than that of naphthalene are not present in the gas stream past the PCS system.

The concentrations of various species in the water condensate from the sample train were normalized to determine rates of evolution in milligrams per kilogram of coal fed to the gasifier. No clear trends with reactor temperature are evident, indicating that for the temperature range covered, the reactor temperature has little effect on the emission rates of wastewater species.

Efforts continued to determine the fate of several of the more volatile trace metal elements present in the feed coal. Closures on arsenic consistently vary between 35% and 70%, suggesting that a significant fraction of this substance is passing undetected from the system, either in the gas phase or adsorbed on fine particles that are not trapped by the cold trap or impingers. Similar results are obtained for lead, for which the closures never exceeded 34%, indicating a higher volatility for this element.

The problem with mercury is reproducibility, rather than failure to detect a portion of the total emitted element. The quantity of this element appearing in the trapped tar and solids varies dramatically from one run to another. In some instances the apparent amount of mercury in one or the other of these streams exceeds the quantity fed in with the coal.

To aid in the formulation of gasifier performance correlations, a simple mathematical model of the fluidized bed gasifier has been developed which considers the gasification process to occur in three stages: instantaneous devolatilization of coal at the top of the fluidized bed, instantaneous combustion of carbon at the bottom of the bed, and steam/carbon gasification and water gas shift reaction in a single perfectly mixed isothermal stage. The model is significant in and of itself, but its particular importance to the project is that it enables the specification of gasifier conditions required to produce a feed to the acid gas removal system with a predetermined flow rate and composition.

Using optimal parameter values, the model was run for all gasifier runs and gave excellent predictions of carbon conversion and dry make gas flow rate. The sweet gas heating value was calculated from experimental results and from model predictions for each run. (The sweet gas is defined as the dry make gas with the CO_2 and H_2S removed.) The error between predicted and measured heating values was less than 5% for all runs.

The model also does a good job of correlating data on the evolution of individual species can be used to predict the composition of the gasifier make gas for a specified set of reactor conditions, and also to study the effects of individual reactor variables on yield.

Results from the acid gas removal system show that refrigerated methanol is an effective solvent for cleaning of gases produced by coal gasification. The removal of CO_2, COS, and H_2S to sufficiently low levels can be achieved with proper choice of operating conditions and effective solvent regeneration.

The presence of several trace sulfur compounds, mercaptans, thiophenes, organic sulfides, and CS_2, complicates the gas cleaning process. These compounds were found to distribute among all exit streams from the AGRS. If no provision is made to treat these sulfur gases, the possibility of their emission into the atmosphere exists and must be dealt with to avoid significant environmental problems.

A wide variety of aliphatic and aromatic hydrocarbons are present in the gas stream fed to the AGRS. The aliphatic hydrocarbons, ranging from methane to butane, cover a wide range of solubilities. Their presence in all AGRS streams must be anticipated to prevent their emission to the atmosphere.

While a wide range of simple aromatics were identified in the gas stream fed to the AGRS, essentially no polynuclear aromatic compounds were found. Apparently, the gas quenching process effectively removes these compounds from the gasifier product gas. However, significant quantities of simple aromatics were found to accumulate in the recirculating methanol increasing the potential for their discharge to the atmosphere. Provision must be made to purge the solvent of these compounds or to remove them prior to the AGRS through cold traps.

In an environmental context, use of refrigerated methanol as an acid gas removal solvent for coal gas cleaning must be accompanied by safeguards to avoid several potential problems. The need for polishing steps on any discharge stream appears necessary because of the wide distribution of several potential pollutants throughout the AGRS. The nature and design of these polishing steps will depend on the required discharge levels of specific pollutants manufactured in the gasification process.

As a part of the AGRS research program, a mathematical model of the absorber has been developed. The model assumes adiabatic operation of the column and uses appropriate mass and energy balances, physical and transport property information, and phase equilibrium relationships to simulate steady-state behavior of the absorber. The model was tested by comparing its predictions with experimental data for runs made with a mixture of nitrogen and carbon dioxide only (syngas runs) and with reactor make gas from the PCS system.

For the syngas runs the measured and predicted liquid temperature profiles showed excellent agreement. For runs using reactor make gas there was very good agreement between the predicted and experimental concentrations for most compounds. However, experimental data and model predictions for H_2S, C_2H_4, and C_2H_6 show some small differences. These differences were shown to be related to the fact that the entering methanol was not adequately stripped and contained some H_2S. The input data to the model assumed that clean methanol was fed to the column. The difference between the values for C_2H_4 and C_2H_6 may be related to the fact that Henry's law does not provide an accurate correlation of vapor-liquid equilibrium data for these species.

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APPENDIX A
GASIFIER-PCS
MASS BALANCE RESULTS

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                 NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                 FLUIDIZED BED COAL GASIFICATION REACTOR

                     RUN GO-62  8-20-80  11:40-13:30

   REACTOR SPECIFICATIONS                  FEED RATES AND RATIOS

  PRESSURE     = 102.1 PSIG           COAL        = 45.00 LB/HR
  TEMPERATURE  = 1805.0 DEG.F         STEAM       = 56.93 LB/HR
  BED HEIGHT   = 38.0 IN.             OXYGEN      = 15.13 LB/HR
  BED DIAMETER =  6.0 IN.             NITROGEN    =  4.49 LB/HR
  ESTIMATED BED VOIDAGE = 0.78        PURGE N2    = 15.39 LB/HR
  SOLIDS HOLDUP = 15.0 LB             H2O/CARBON  = 1.09 MOLES H2O/MOLE C
                                      O2/CARBON   = 0.16 MOLES O2/MOLE C
                                      N2/O2       = 0.34 MOLES N2/MOLE O2

              ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                   MASS      C       H       O       N       S

        COAL       45.0    34.77   0.48    2.48    0.23   1.126
        GASES      91.9     0.00   6.37   65.68   19.89   0.000
  TOTAL INPUT     136.9    34.77   6.85   68.16   20.11   1.126

        CHAR       21.3    15.76   0.10    0.44    0.11   0.413
        DUST        2.0     0.98   0.01    0.19    0.01   0.028
        GASES     116.1    13.59   7.64   74.15   19.99   0.716
   WASTEWATER       0.0     0.00   0.00    0.00    0.00   0.000
 TOTAL OUTPUT     139.4    30.32   7.75   74.78   20.11   1.157

 % RECOVERY      101.8%    87.2%  113.2%  109.7%  100.0%  102.8%


                     OUTPUT VARIABLES

          CARBON CONVERSION (PERCENT)               39.1
          DRY MAKE GAS FLOW RATE (SCFM)             15.6
          HEATING VALUE OF SWEET GAS (BTU/SCF)     332.8
          EFFLUENT FLOW RATES (LB/HR)
                   CO                              12.00
                   H2                               1.46
                   CH4                              0.98
                   CO2                             28.21
                   N2                              19.99
                   H2S                              0.735
                   COS                              0.047
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                     NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                     FLUIDIZED BED COAL GASIFICATION REACTOR

                         RUN GO-62  8-20-80  11:40-13:30

  REACTOR SPECIFICATIONS                   FEED RATES AND RATIOS

PRESSURE     = 805.1 KPA                COAL       = 20.41 KG/HR
TEMPERATURE  =  985.0 DEG.C             STEAM      = 25.82 KG/HR
BED HEIGHT   = 0.97 METERS              OXYGEN     =  6.86 KG/HR
BED DIAMETER = 0.152 METERS             NITROGEN   =  2.04 KG/HR
ESTIMATED BED VOIDAGE = 0.78            PURGE N2   =  6.98 KG/HR
SOLIDS HOLDUP = 6.8 KG                  H2O/CARBON = 1.09 MOLES H2O/MOLE C
                                        O2/CARBON  = 0.16 MOLES O2/MOLE C
                                        N2/O2      = 0.34 MOLES N2/MOLE O2


                     ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

                         MASS       C        H        O        N        S

               COAL      20.4    15.77     0.22     1.12     0.10    0.511
               GASES     41.7     0.00     2.89    29.79     9.02    0.000
        TOTAL INPUT      62.1    15.77     3.10    30.92     9.12    0.511

               CHAR       9.7     7.15     0.04     0.20     0.05    0.187
               DUST       0.9     0.44     0.01     0.08     0.00    0.013
               GASES     52.7     6.16     3.46    33.63     9.07    0.325
         WASTEWATER       0.0     0.00     0.00     0.00     0.00    0.000
       TOTAL OUTPUT      63.2    13.75     3.52    33.92     9.12    0.525

       % RECOVERY      101.8%    87.2%   113.2%   109.7%   100.0%   102.8%


                             OUTPUT VARIABLES

               CARBON CONVERSION (PERCENT)              39.1
               DRY MAKE GAS FLOW RATE (SCMM)            0.44
               HEATING VALUE OF SWEET GAS (KJ/SCM)     12400
               EFFLUENT FLOW RATES (KG/HR)
                         CO                             5.44
                         H2                             0.66
                         CH4                            0.44
                         CO2                           12.80
                         N2                             9.07
                         H2S                            0.333
                         COS                            0.021
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                 NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                 FLUIDIZED BED COAL GASIFICATION REACTOR

                     RUN GO-63B  9-3-80  11:00-12:15

  REACTOR SPECIFICATIONS                 FEED RATES AND RATIOS

PRESSURE     = 103.0 PSIG             COAL       = 39.00 LB/HR
TEMPERATURE  = 1816.4 DEG.F           STEAM      = 56.45 LB/HR
BED HEIGHT   = 38.0 IN.               OXYGEN     = 14.33 LB/HR
BED DIAMETER =  6.0 IN.               NITROGEN   =  4.63 LB/HR
ESTIMATED BED VOIDAGE = 0.75          PURGE N2   =  9.57 LB/HR
SOLIDS HOLDUP = 15.7 LB               H2O/CARBON = 1.34 MOLES H2O/MOLE C
                                      O2/CARBON  = 0.19 MOLES O2/MOLE C
                                      N2/O2      = 0.37 MOLES N2/MOLE O2


               ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                   MASS      C        H        O        N        S

          COAL     39.0    28.12     0.70     3.13     0.20    0.887
         GASES     85.0     0.00     6.32    64.45    14.21    0.000
   TOTAL INPUT    124.0    28.12     7.01    67.59    14.40    0.887

          CHAR     14.7     9.30     0.05     0.74     0.07    0.216
          DUST      1.9     1.31     0.01     0.10     0.01    0.021
         GASES    106.6    16.57     6.76    68.34    14.32    0.599
    WASTEWATER      0.0     0.00     0.00     0.00     0.00    0.000
  TOTAL OUTPUT    123.2    27.18     6.82    69.18    14.40    0.836

  % RECOVERY      99.3%    96.6%    97.3%   102.4%   100.0%    94.2%


                         OUTPUT VARIABLES

          CARBON CONVERSION (PERCENT)            58.9
          DRY MAKE GAS FLOW RATE (SCFM)          16.7
          HEATING VALUE OF SWEET GAS (BTU/SCF)  348.5
          EFFLUENT FLOW RATES (LB/HR)
                    CO                          15.88
                    H2                           1.76
                    CH4                          1.55
                    CO2                         31.48
                    N2                          14.32
                    H2S                          0.611
                    COS                          0.045
                 NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                 FLUIDIZED BED COAL GASIFICATION REACTOR


                     RUN GO-63B  9-3-80  11:00-12:15

  REACTOR SPECIFICATIONS                 FEED RATES AND RATIOS

 PRESSURE     = 811.4 KPA             COAL        = 17.69 KG/HR
 TEMPERATURE  =  991.3 DEG.C          STEAM       = 25.61 KG/HR
 BED HEIGHT   = 0.97 METERS           OXYGEN      =  6.50 KG/HR
 BED DIAMETER = 0.152 METERS          NITROGEN    =  2.10 KG/HR
 ESTIMATED BED VOIDAGE = 0.75         PURGE N2    =  4.34 KG/HR
 SOLIDS HOLDUP = 7.1 KG               H2O/CARBON = 1.34 MOLES H2O/MOLE C
                                      O2/CARBON  = 0.19 MOLES O2/MOLE C
                                      N2/O2      = 0.37 MOLES N2/MOLE O2


                 ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

                     MASS     C        H        O        N        S

         COAL        17.7   12.76     0.32     1.42     0.09    0.403
         GASES       38.5    0.00     2.86    29.24     6.44    0.000
   TOTAL INPUT       56.2   12.76     3.18    30.66     6.53    0.403

         CHAR         6.6    4.22     0.02     0.34     0.03    0.098
         DUST         0.9    0.59     0.01     0.05     0.00    0.009
         GASES       48.4    7.51     3.07    31.00     6.50    0.272
    WASTEWATER        0.0    0.00     0.00     0.00     0.00    0.000
  TOTAL OUTPUT       55.9   12.33     3.10    31.38     6.53    0.379

  % RECOVERY        99.3%   96.6%    97.3%   102.4%   100.0%    94.2%


                         OUTPUT VARIABLES

         CARBON CONVERSION (PERCENT)                  58.9
         DRY MAKE GAS FLOW RATE (SCMM)                0.47
         HEATING VALUE OF SWEET GAS (KJ/SCM)         12982
         EFFLUENT FLOW RATES (KG/HR)
                   CO                                 7.20
                   H2                                 0.80
                   CH4                                0.70
                   CO2                               14.28
                   N2                                 6.50
                   H2S                                0.277
                   COS                                0.020
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                NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                FLUIDIZED BED COAL GASIFICATION REACTOR

                    RUN GO-64  9-25-80  11:00-14:00

  REACTOR SPECIFICATIONS                 FEED RATES AND RATIOS

PRESSURE     = 102.7 PSIG             COAL       = 41.41 LB/HR
TEMPERATURE  = 1802.1 DEG.F           STEAM      = 57.28 LB/HR
BED HEIGHT   = 38.0 IN.               OXYGEN     = 14.33 LB/HR
BED DIAMETER =  6.0 IN.               NITROGEN   =  5.48 LB/HR
ESTIMATED BED VOIDAGE = 0.75          PURGE N2   =  8.34 LB/HR
SOLIDS HOLDUP = 14.8 LB               H2O/CARBON = 1.36 MOLES H2O/MOLE C
                                      O2/CARBON  = 0.19 MOLES O2/MOLE C
                                      N2/O2      = 0.44 MOLES N2/MOLE O2

              ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                  MASS      C        H        O        N        S

         COAL     41.4    28.10     1.08     2.41     0.21    0.765
        GASES     85.4     0.00     6.41    65.19    13.82    0.000
  TOTAL INPUT    126.8    28.10     7.49    67.60    14.03    0.765

         CHAR     13.1     8.03     0.06     0.03     0.07    0.200
         DUST      3.2     1.89     0.02     0.10     0.02    0.023
        GASES    114.5    17.78     7.32    74.87    13.95    0.570
   WASTEWATER      0.0     0.00     0.00     0.00     0.00    0.000
 TOTAL OUTPUT    130.8    27.69     7.40    75.00    14.03    0.793

 % RECOVERY    103.1%    98.5%    98.8%   111.0%   100.0%   103.6%


                      OUTPUT VARIABLES

          CARBON CONVERSION (PERCENT)              63.2
          DRY MAKE GAS FLOW RATE (SCFM)            16.9
          HEATING VALUE OF SWEET GAS (BTU/SCF)    357.7
          EFFLUENT FLOW RATES (LB/HR)
                    CO                             15.26
                    H2                              1.65
                    CH4                             2.13
                    CO2                            35.30
                    N2                             13.95
                    H2S                             0.581
                    COS                             0.043
              NCSU DEPARTMENT OF CHEMICAL ENGINEERING

              FLUIDIZED BED COAL GASIFICATION REACTOR

                  RUN GO-64  9-25-80  11:00-14:00

  REACTOR SPECIFICATIONS              FEED RATES AND RATIOS

PRESSURE     = 809.7 KPA           COAL       = 18.78 KG/HR
TEMPERATURE  =  983.4 DEG.C        STEAM      = 25.98 KG/HR
BED HEIGHT   = 0.97 METERS         OXYGEN     =  6.50 KG/HR
BED DIAMETER = 0.152 METERS        NITROGEN   =  2.48 KG/HR
ESTIMATED BED VOIDAGE = 0.75       PURGE N2   =  3.78 KG/HR
SOLIDS HOLDUP = 6.7 KG             H2O/CARBON = 1.36 MOLES H2O/MOLE C
                                   O2/CARBON  = 0.19 MOLES O2/MOLE C
                                   N2/O2      = 0.44 MOLES N2/MOLE O2

              ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

                  MASS      C       H       O       N       S

          COAL    18.8   12.75    0.49    1.09    0.09   0.347
         GASES    38.7    0.00    2.91   29.57    6.27   0.000
    TOTAL INPUT   57.5   12.75    3.40   30.66    6.36   0.347

          CHAR     6.0    3.64    0.03    0.02    0.03   0.091
          DUST     1.5    0.86    0.01    0.04    0.01   0.011
         GASES    51.9    8.06    3.32   33.96    6.33   0.258
    WASTEWATER     0.0    0.00    0.00    0.00    0.00   0.000
   TOTAL OUTPUT   59.3   12.56    3.36   34.02    6.36   0.360

   % RECOVERY   103.1%   98.5%   98.8%  111.0%  100.0%  103.6%


                      OUTPUT VARIABLES

          CARBON CONVERSION (PERCENT)             63.2
          DRY MAKE GAS FLOW RATE (SCMM)           0.48
          HEATING VALUE OF SWEET GAS (KJ/SCM)    13326
          EFFLUENT FLOW RATES (KG/HR)
                    CO                            6.92
                    H2                            0.75
                    CH4                           0.96
                    CO2                          16.01
                    N2                            6.33
                    H2S                           0.263
                    COS                           0.020
                    NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                    FLUIDIZED BED COAL GASIFICATION REACTOR


                        RUN GO-65  10-2-80  11:00-13:00

   REACTOR SPECIFICATIONS                   FEED RATES AND RATIOS

  PRESSURE     = 102.5 PSIG               COAL        = 48.33 LB/HR
  TEMPERATURE  = 1707.1 DEG.F             STEAM       = 59.92 LB/HR
  BED HEIGHT   = 38.0 IN.                 OXYGEN      = 13.47 LB/HR
  BED DIAMETER =  6.0 IN.                 NITROGEN    =  5.29 LB/HR
  ESTIMATED BED VOIDAGE = 0.74            PURGE N2    =  9.15 LB/HR
  SOLIDS HOLDUP = 15.6 LB                 H2O/CARBON = 1.27 MOLES H2O/MOLE C
                                          O2/CARBON  = 0.16 MOLES O2/MOLE C
                                          N2/O2      = 0.45 MOLES N2/MOLE O2


                    ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                        MASS      C        H        O        N        S

             COAL       48.3    31.57     1.31     6.02     0.24    0.825
             GASES      87.8     0.00     6.70    66.68    14.44    0.000
     TOTAL INPUT       136.2    31.57     8.01    72.70    14.68    0.825

             CHAR       21.8    15.83     0.10     0.32     0.11    0.382
             DUST        2.6     1.52     0.02     0.27     0.01    0.020
             GASES     111.2    15.96     7.39    72.81    14.55    0.492
       WASTEWATER        0.0     0.00     0.00     0.00     0.00    0.000
     TOTAL OUTPUT      135.6    33.31     7.51    73.41    14.67    0.894

     % RECOVERY        99.6%   105.5%    93.7%   101.0%   100.0%   108.4%


                            OUTPUT VARIABLES

             CARBON CONVERSION (PERCENT)               50.6
             DRY MAKE GAS FLOW RATE (SCFM)             15.6
             HEATING VALUE OF SWEET GAS (BTU/SCF)     375.0
             EFFLUENT FLOW RATES (LB/HR)
                  CO                                  11.02
                  H2                                   1.47
                  CH4                                  2.55
                  CO2                                 34.15
                  N2                                  14.55
                  H2S                                  0.507
                  COS                                  0.027
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NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-65 10-2-80 11:00-13:00

REACTOR SPECIFICATIONS

PRESSURE = 808.0 KPA
TEMPERATURE = 930.6 DEG.C
BED HEIGHT = 0.97 METERS
BED DIAMETER = 0.152 METERS
ESTIMATED BED VOIDAGE = 0.74
SOLIDS HOLDUP = 7.1 KG

FEED RATES AND RATIOS

COAL = 21.92 KG/HR
STEAM = 27.18 KG/HR
OXYGEN = 6.11 KG/HR
NITROGEN = 2.40 KG/HR
PURGE N2 = 4.15 KG/HR
H2O/CARBON = 1.27 MOLES H2O/MOLE C
O2/CARBON = 0.16 MOLES O2/MOLE C
N2/O2 = 0.45 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

	MASS	C	H	O	N	S
COAL	21.9	14.32	0.59	2.73	0.11	0.374
GASES	39.8	0.00	3.04	30.24	6.55	0.000
TOTAL INPUT	61.8	14.32	3.63	32.98	6.66	0.374
CHAR	9.9	7.18	0.04	0.15	0.05	0.173
DUST	1.2	0.69	0.01	0.12	0.01	0.009
GASES	50.4	7.24	3.35	33.03	6.60	0.223
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	61.5	15.11	3.41	33.30	6.66	0.405
% RECOVERY	99.6%	105.5%	93.7%	101.0%	100.0%	108.4%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	50.6
DRY MAKE GAS FLOW RATE (SCMM)	0.44
HEATINC VALUE OF SWEET GAS (KJ/SCM)	13969
EFFLUENT FLOW RATES (KG/HR)	
CO	5.00
H2	0.67
CH4	1.16
CO2	15.49
N2	6.60
H2S	0.230
COS	0.012

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                 NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                 FLUIDIZED BED COAL GASIFICATION REACTOR


                     RUN GO-66  10-21-80  11:30-13:00


   REACTOR SPECIFICATIONS                  FEED RATES AND RATIOS

  PRESSURE     = 103.6 PSIG               COAL      = 42.64 LB/HR
  TEMPERATURE  = 1798.5 DEG.F             STEAM     = 57.30 LB/HR
  BED HEIGHT   = 38.0 IN.                 OXYGEN    = 17.80 LB/HR
  BED DIAMETER =  6.0 IN.                 NITROGEN  =  5.29 LB/HR
  ESTIMATED BED VOIDAGE = 0.74            PURGE N2  =  9.06 LB/HR
  SOLIDS HOLDUP = 13.5 LB                 H2O/CARBON = 1.69 MOLES H2O/MOLE C
                                          O2/CARBON  = 0.30 MOLES O2/MOLE C
                                          N2/O2      = 0.34 MOLES N2/MOLE O2


                 ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                     MASS      C        H        O        N        S

           COAL      42.6    22.58     2.00     8.83     0.21    0.322
          GASES      89.5     0.00     6.41    68.68    14.35    0.000
    TOTAL INPUT     132.1    22.58     8.41    77.51    14.57    0.322

           CHAR       5.4     1.17     0.06     0.19     0.03    0.043
           DUST       0.1     0.05     0.00     0.01     0.00    0.000
          GASES     125.4    21.87     8.31    80.33    14.55    0.345
     WASTEWATER       0.0     0.00     0.00     0.00     0.00    0.000
   TOTAL OUTPUT     130.9    23.09     8.38    80.53    14.57    0.388

   % RECOVERY       99.1%   102.2%    99.6%   103.9%   100.0%   120.4%


                        OUTPUT VARIABLES

           CARBON CONVERSION (PERCENT)             96.8
           DRY MAKE GAS FLOW RATE (SCFM)           19.8
           HEATING VALUE OF SWEET GAS (BTU/SCF)   407.1
           EFFLUENT FLOW RATES (LB/HR)
                     CO                           18.65
                     H2                            1.90
                     CH4                           4.51
                     CO2                          38.43
                     N2                           14.55
                     H2S                           0.353
                     COS                           0.024
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NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-66 10-21-80 11:30-13:00

REACTOR SPECIFICATIONS

PRESSURE = 815.9 KPA
TEMPERATURE = 981.4 DEG.C
BED HEIGHT = 0.97 METERS
BED DIAMETER = 0.152 METERS
ESTIMATED BED VOIDAGE = 0.74
SOLIDS HOLDUP = 6.1 KG

FEED RATES AND RATIOS

COAL = 19.34 KG/HR
STEAM = 25.99 KG/HR
OXYGEN = 8.07 KG/HR
NITROGEN = 2.40 KG/HR
PURGE N2 = 4.11 KG/HR
H2O/CARBON = 1.69 MOLES H2O/MOLE C
O2/CARBON = 0.30 MOLES O2/MOLE C
N2/O2 = 0.34 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

	MASS	C	H	O	N	S
COAL	19.3	10.24	0.91	4.00	0.10	0.146
GASES	40.6	0.00	2.91	31.15	6.51	0.000
TOTAL INPUT	59.9	10.24	3.82	35.16	6.61	0.146
CHAR	2.4	0.53	0.03	0.09	0.01	0.020
DUST	0.0	0.02	0.00	0.00	0.00	0.000
GASES	56.9	9.92	3.77	36.44	6.60	0.156
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	59.4	10.47	3.80	36.53	6.61	0.176
% RECOVERY	99.1%	102.2%	99.6%	103.9%	100.0%	120.4%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	96.8
DRY MAKE GAS FLOW RATE (SCMM)	0.56
HEATING VALUE OF SWEET GAS (KJ/SCM)	15165
EFFLUENT FLOW RATES (KG/HR)	
CO	8.46
H2	0.86
CH4	2.05
CO2	17.43
N2	6.60
H2S	0.160
COS	0.011

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                NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                FLUIDIZED BED COAL GASIFICATION REACTOR


                    RUN GO-68B  11-19-80  14:00-16:30


   REACTOR SPECIFICATIONS               FEED RATES AND RATIOS

 PRESSURE     = 105.0 PSIG          COAL       = 63.60 LB/HR
 TEMPERATURE  = 1786.5 DEG.F        STEAM      = 56.83 LB/HR
 BED HEIGHT   = 38.0 IN.            OXYGEN     = 17.64 LB/HR
 BED DIAMETER =  6.0 IN.            NITROGEN   =  6.27 LB/HR
 ESTIMATED BED VOIDAGE = 0.80       PURGE N2   = 13.69 LB/HR
 SOLIDS HOLDUP = 10.4 LB            H2O/CARBON = 1.12 MOLES H2O/MOLE C
                                    O2/CARBON  = 0.20 MOLES O2/MOLE C
                                    N2/O2      = 0.41 MOLES N2/MOLE O2


                ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                    MASS      C       H       O       N       S

         COAL       63.6    33.69    2.99   13.17    0.32   0.481
         GASES      94.4     0.00    6.36   68.11   19.96   0.000
   TOTAL INPUT     158.0    33.69    9.35   81.27   20.28   0.481

         CHAR       19.4     7.88    0.34    1.79    0.10   0.117
         DUST        4.5     1.23    0.03    0.05    0.02   0.014
         GASES     130.8    22.47    8.69   79.14   20.16   0.330
    WASTEWATER       0.0     0.00    0.00    0.00    0.00   0.000
  TOTAL OUTPUT     154.6    31.59    9.06   80.98   20.28   0.461

  % RECOVERY       97.9%    93.8%   97.0%   99.6%  100.0%   95.8%


                         OUTPUT VARIABLES

         CARBON CONVERSION (PERCENT)               66.7
         DRY MAKE GAS FLOW RATE (SCFM)             23.3
         HEATING VALUE OF SWEET GAS (BTU/SCF)     381.1
         EFFLUENT FLOW RATES (LB/HR)
                   CO                              23.08
                   H2                               2.57
                   CH4                              4.02
                   CO2                             35.06
                   N2                              20.16
                   H2S                              0.335
                   COS                              0.027
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                 NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                 FLUIDIZED BED COAL GASIFICATION REACTOR


                     RUN GO-68B  11-19-80  14:00-16:30

  REACTOR SPECIFICATIONS                FEED RATES AND RATIOS

PRESSURE     = 825.2 KPA             COAL       = 28.85 KG/HR
TEMPERATURE  =  974.7 DEG.C          STEAM      = 25.78 KG/HR
BED HEIGHT   = 0.97 METERS           OXYGEN     =  8.00 KG/HR
BED DIAMETER = 0.152 METERS          NITROGEN   =  2.84 KG/HR
ESTIMATED BED VOIDAGE = 0.80         PURGE N2   =  6.21 KG/HR
SOLIDS HOLDUP = 4.7 KG               H2O/CARBON = 1.12 MOLES H2O/MOLE C
                                     O2/CARBON  = 0.20 MOLES O2/MOLE C
                                     N2/O2      = 0.41 MOLES N2/MOLE O2


             ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

                 MASS     C        H        O        N        S

        COAL     28.8   15.28     1.36     5.97     0.15    0.218
       GASES     42.8    0.00     2.88    30.89     9.05    0.000
 TOTAL INPUT     71.7   15.28     4.24    36.87     9.20    0.218

        CHAR      8.8    3.57     0.16     0.81     0.04    0.053
        DUST      2.0    0.56     0.01     0.02     0.01    0.007
       GASES     59.3   10.19     3.94    35.90     9.15    0.150
  WASTEWATER      0.0    0.00     0.00     0.00     0.00    0.000
TOTAL OUTPUT     70.1   14.33     4.11    36.73     9.20    0.209

% RECOVERY      97.9%   93.8%    97.0%    99.6%   100.0%    95.8%



                         OUTPUT VARIABLES

        CARBON CONVERSION (PERCENT)                66.7
        DRY MAKE GAS FLOW RATE (SCMM)              0.66
        HEATING VALUE OF SWEET GAS (KJ/SCM)       14199
        EFFLUENT FLOW RATES (KG/HR)
                  CO                              10.47
                  H2                               1.17
                  CH4                              1.82
                  CO2                             15.90
                  N2                               9.15
                  H2S                              0.152
                  COS                              0.012
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NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-69B 12-15-80 13:30-16:00

REACTOR SPECIFICATIONS

PRESSURE = 105.8 PSIG
TEMPERATURE = 1720.2 DEG.F
BED HEIGHT = 38.0 IN.
BED DIAMETER = 6.0 IN.
ESTIMATED BED VOIDAGE = 0.84
SOLIDS HOLDUP = 8.4 LB

FEED RATES AND RATIOS

COAL = 54.83 LB/HR
STEAM = 56.71 LB/HR
OXYGEN = 15.50 LB/HR
NITROGEN = 8.19 LB/HR
PURGE N2 = 13.87 LB/HR
H2O/CARBON = 1.56 MOLES H2O/MOLE C
O2/CARBON = 0.24 MOLES O2/MOLE C
N2/O2 = 0.60 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

	MASS	C	H	O	N	S
COAL	54.8	24.22	2.01	11.42	0.46	0.457
GASES	94.3	0.00	6.34	65.86	22.06	0.000
TOTAL INPUT	149.1	24.22	8.35	77.28	22.52	0.457
CHAR	22.0	7.01	0.11	1.70	0.09	0.113
DUST	0.0	0.00	0.00	0.00	0.00	0.000
GASES	122.3	16.59	8.53	74.40	22.44	0.297
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	144.3	23.60	8.64	76.11	22.52	0.410
% RECOVERY	96.8%	97.4%	103.4%	98.5%	100.0%	89.9%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	68.5
DRY MAKE GAS FLOW RATE (SCFM)	18.9
HEATING VALUE OF SWEET GAS (BTU/SCF)	376.2
EFFLUENT FLOW RATES (LB/HR)	
CO	12.24
H2	1.92
CH4	3.79
CO2	31.15
N2	22.44
H2S	0.308
COS	0.014

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                NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                FLUIDIZED BED COAL GASIFICATION REACTOR


                    RUN GO-69B  12-15-80  13:30-16:00

   REACTOR SPECIFICATIONS                  FEED RATES AND RATIOS

 PRESSURE     = 830.8 KPA               COAL       = 24.87 KG/HR
 TEMPERATURE  =  937.9 DEG.C            STEAM      = 25.72 KG/HR
 BED HEIGHT   = 0.97 METERS             OXYGEN     =  7.03 KG/HR
 BED DIAMETER = 0.152 METERS            NITROGEN   =  3.72 KG/HR
 ESTIMATED BED VOIDAGE = 0.84           PURGE N2   =  6.29 KG/HR
 SOLIDS HOLDUP = 3.8 KG                 H2O/CARBON = 1.56 MOLES H2O/MOLE C
                                        O2/CARBON  = 0.24 MOLES O2/MOLE C
                                        N2/O2      = 0.60 MOLES N2/MOLE O2


             ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

                    MASS      C        H        O        N        S

           COAL     24.9    10.99     0.91     5.18     0.21    0.207
          GASES     42.8     0.00     2.88    29.87    10.01    0.000
    TOTAL INPUT     67.6    10.99     3.79    35.06    10.21    0.207

           CHAR     10.0     3.18     0.05     0.77     0.04    0.051
           DUST      0.0     0.00     0.00     0.00     0.00    0.000
          GASES     55.5     7.53     3.87    33.75    10.18    0.135
     WASTEWATER      0.0     0.00     0.00     0.00     0.00    0.000
   TOTAL OUTPUT     65.4    10.70     3.92    34.52    10.22    0.186

   % RECOVERY      96.8%    97.4%   103.4%    98.5%   100.0%    89.9%


                         OUTPUT VARIABLES

          CARBON CONVERSION (PERCENT)              68.5
          DRY MAKE GAS FLOW RATE (SCMM)            0.53
          HEATING VALUE OF SWEET GAS (KJ/SCM)     14017
          EFFLUENT FLOW RATES (KG/HR)
                    CO                             5.55
                    H2                             0.87
                    CH4                            1.72
                    CO2                           14.13
                    N2                            10.18
                    H2S                            0.140
                    COS                            0.007
                NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                FLUIDIZED BED COAL GASIFICATION REACTOR

                    RUN GO-70  1-8-81  14:00-16:30

    REACTOR SPECIFICATIONS                FEED RATES AND RATIOS

  PRESSURE     = 105.8 PSIG            COAL       = 48.38 LB/HR
  TEMPERATURE  = 1781.1 DEG.F          STEAM      = 57.61 LB/HR
  BED HEIGHT   = 38.0 IN.              OXYGEN     = 16.79 LB/HR
  BED DIAMETER =  6.0 IN.              NITROGEN   =  5.62 LB/HR
  ESTIMATED BED VOIDAGE = 0.97         PURGE N2   = 14.87 LB/HR
  SOLIDS HOLDUP =  1.8 LB              H2O/CARBON = 1.81 MOLES H2O/MOLE C
                                       O2/CARBON  = 0.30 MOLES O2/MOLE C
                                       N2/O2      = 0.38 MOLES N2/MOLE O2

               ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                    MASS      C       H       O       N       S

           COAL     48.4    21.24    1.77   10.92    0.24   0.383
          GASES     94.9     0.00    6.45   67.94   20.49   0.000
    TOTAL INPUT    143.3    21.24    8.21   78.86   20.73   0.383

           CHAR     13.3     1.00    0.03    0.10    0.01   0.061
           DUST      2.7     1.44    0.02    0.46    0.01   0.008
          GASES    120.5    18.24    8.11   73.20   20.71   0.264
     WASTEWATER      0.0     0.00    0.00    0.00    0.00   0.000
   TOTAL OUTPUT    136.5    20.67    8.17   73.76   20.74   0.333

   % RECOVERY      95.3%    97.3%   99.4%   93.5%  100.1%   87.0%


                    OUTPUT VARIABLES

            CARBON CONVERSION (PERCENT)            85.9
            DRY MAKE GAS FLOW RATE (SCFM)          20.0
            HEATING VALUE OF SWEET GAS (BTU/SCF)  379.4
            EFFLUENT FLOW RATES (LB/HR)
                      CO                           16.76
                      H2                            2.13
                      CH4                           3.31
                      CO2                          31.40
                      N2                           20.71
                      H2S                           0.272
                      COS                           0.015
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NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-70 1-8-81 14:00-16:30

REACTOR SPECIFICATIONS

PRESSURE = 831.1 KPA
TEMPERATURE = 971.8 DEG.C
BED HEIGHT = 0.97 METERS
BED DIAMETER = 0.152 METERS
ESTIMATED BED VOIDAGE = 0.97
SOLIDS HOLDUP = 0.8 KG

FEED RATES AND RATIOS

COAL = 21.94 KG/HR
STEAM = 26.13 KG/HR
OXYGEN = 7.61 KG/HR
NITROGEN = 2.55 KG/HR
PURGE N_2 = 6.75 KG/HR
H_2O/CARBON = 1.81 MOLES H_2O/MOLE C
O_2/CARBON = 0.30 MOLES O_2/MOLE C
N_2/O_2 = 0.38 MOLES N_2/MOLE O_2

ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

	MASS	C	H	O	N	S
COAL	21.9	9.63	0.80	4.95	0.11	0.174
GASES	43.0	0.00	2.92	30.82	9.29	0.000
TOTAL INPUT	65.0	9.63	3.72	35.77	9.40	0.174
CHAR	6.0	0.45	0.01	0.05	0.01	0.028
DUST	1.2	0.65	0.01	0.21	0.01	0.004
GASES	54.7	8.27	3.68	33.20	9.40	0.120
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	61.9	9.38	3.70	33.46	9.41	0.151
% RECOVERY	95.3%	97.3%	99.4%	93.5%	100.1%	87.0%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	85.9
DRY MAKE GAS FLOW RATE (SCMM)	0.56
HEATING VALUE OF SWEET GAS (KJ/SCM)	14133
EFFLUENT FLOW RATES (KG/HR)	
CO	7.60
H_2	0.97
CH_4	1.50
CO_2	14.24
N_2	9.40
H_2S	0.123
COS	0.007

NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-71B 1-27-81 14:30-15:30

REACTOR SPECIFICATIONS

PRESSURE = 105.2 PSIG
TEMPERATURE = 1798.4 DEG.F
BED HEIGHT = 38.0 IN.
BED DIAMETER = 6.0 IN.
ESTIMATED BED VOIDAGE = 0.76
SOLIDS HOLDUP = 12.3 LB

FEED RATES AND RATIOS

COAL = 45.81 LB/HR
STEAM = 57.28 LB/HR
OXYGEN = 16.04 LB/HR
NITROGEN = 5.80 LB/HR
PURGE N2 = 11.45 LB/HR
H2O/CARBON = 1.65 MOLES H2O/MOLE C
O2/CARBON = 0.26 MOLES O2/MOLE C
N2/O2 = 0.41 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

	MASS	C	H	O	N	S
COAL	45.8	23.19	1.91	10.44	0.46	0.372
GASES	90.6	0.00	6.41	66.90	17.25	0.000
TOTAL INPUT	136.4	23.19	8.32	77.34	17.71	0.372
CHAR	13.0	0.78	0.04	0.10	0.06	0.065
DUST	2.8	1.18	0.03	0.11	0.01	0.008
GASES	125.4	20.83	8.77	77.59	17.78	0.439
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	141.2	22.79	8.84	77.79	17.86	0.512
% RECOVERY	103.5%	98.3%	106.2%	100.6%	100.8%	137.6%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	89.8
DRY MAKE GAS FLOW RATE (SCFM)	21.8
HEATING VALUE OF SWEET GAS (BTU/SCF)	385.4
EFFLUENT FLOW RATES (LB/HR)	
CO	19.37
H2	2.53
CH4	4.07
CO2	34.72
N2	17.78
H2S	0.452
COS	0.026

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                    NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                    FLUIDIZED BED COAL GASIFICATION REACTOR


                        RUN GO-71B  1-27-81  14:30-15:30


  REACTOR SPECIFICATIONS                  FEED RATES AND RATIOS

PRESSURE     = 826.7 KPA              COAL       = 20.78 KG/HR
TEMPERATURE  =  981.3 DEG.C           STEAM      = 25.98 KG/HR
BED HEIGHT   = 0.97 METERS            OXYGEN     =  7.27 KG/HR
BED DIAMETER = 0.152 METERS           NITROGEN   =  2.63 KG/HR
ESTIMATED BED VOIDAGE = 0.76          PURGE N2   =  5.19 KG/HR
SOLIDS HOLDUP = 5.6 KG                H2O/CARBON = 1.65 MOLES H2O/MOLE C
                                      O2/CARBON  = 0.26 MOLES O2/MOLE C
                                      N2/O2      = 0.41 MOLES N2/MOLE O2


               ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

                   MASS      C       H       O       N       S

          COAL     20.8    10.52    0.87    4.73    0.21   0.169
         GASES     41.1     0.00    2.91   30.35    7.83   0.000
   TOTAL INPUT     61.9    10.52    3.78   35.08    8.04   0.169

          CHAR      5.9     0.35    0.02    0.04    0.03   0.029
          DUST      1.3     0.54    0.01    0.05    0.01   0.003
         GASES     56.9     9.45    3.98   35.19    8.07   0.199
    WASTEWATER      0.0     0.00    0.00    0.00    0.00   0.000
  TOTAL OUTPUT     64.0    10.34    4.01   35.29    8.10   0.232

  % RECOVERY     103.5%    98.3%  106.2%  100.6%  100.8%  137.6%


                            OUTPUT VARIABLES

          CARBON CONVERSION (PERCENT)                89.8
          DRY MAKE GAS FLOW RATE (SCMM)              0.62
          HEATING VALUE OF SWEET GAS (KJ/SCM)       14359
          EFFLUENT FLOW RATES (KG/HR)
                    CO                               8.78
                    H2                               1.15
                    CH4                              1.84
                    CO2                             15.75
                    N2                               8.07
                    H2S                              0.205
                    COS                              0.012
               NCSU DEPARTMENT OF CHEMICAL ENGINEERING

               FLUIDIZED BED COAL GASIFICATION REACTOR


                    RUN GO-72  2-19-81  12:30-14:30


    REACTOR SPECIFICATIONS                 FEED RATES AND RATIOS

   PRESSURE      = 104.4 PSIG           COAL        = 42.33 LB/HR
   TEMPERATURE   = 1797.3 DEG.F         STEAM       = 57.29 LB/HR
   BED HEIGHT    = 38.0 IN.             OXYGEN      = 13.69 LB/HR
   BED DIAMETER  =  6.0 IN.             NITROGEN    =  5.99 LB/HR
   ESTIMATED BED VOIDAGE = 0.70         PURGE N2    = 12.56 LB/HR
   SOLIDS HOLDUP = 15.1 LB              H2O/CARBON  = 1.72 MOLES H2O/MOLE C
                                        O2/CARBON   = 0.23 MOLES O2/MOLE C
                                        N2/O2       = 0.50 MOLES N2/MOLE O2


               ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                    MASS      C       H       O       N       S

            COAL    42.3   22.15    1.77    8.40    0.49   0.335
           GASES    89.5    0.00    6.41   64.56   18.55   0.000
     TOTAL INPUT   131.9   22.15    8.17   72.96   19.04   0.335

            CHAR     7.0    2.90    0.11    0.22    0.06   0.047
            DUST     3.1    0.69    0.12    0.15    0.01   0.007
           GASES   120.1   18.18    8.22   74.33   18.99   0.356
      WASTEWATER     0.0    0.00    0.00    0.00    0.00   0.000
    TOTAL OUTPUT   130.2   21.77    8.45   74.71   19.06   0.410

     % RECOVERY    98.7%   98.3%  103.3%  102.4%  100.1%  122.3%


                          OUTPUT VARIABLES

             CARBON CONVERSION (PERCENT)              82.1
             DRY MAKE GAS FLOW RATE (SCFM)            19.5
             HEATING VALUE OF SWEET GAS (BTU/SCF)    375.2
             EFFLUENT FLOW RATES (LB/HR)
                         CO                           16.45
                         H2                            2.11
                         CH4                           3.27
                         CO2                          31.80
                         N2                           18.99
                         H2S                           0.370
                         COS                           0.015
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                 NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                 FLUIDIZED BED COAL GASIFICATION REACTOR


                     RUN GO-72  2-19-81  12:30-14:30


 REACTOR SPECIFICATIONS                    FEED RATES AND RATIOS

PRESSURE      = 821.4 KPA               COAL        = 19.20 KG/HR
TEMPERATURE   =  980.7 DEG.C            STEAM       = 25.99 KG/HR
BED HEIGHT    = 0.97 METERS             OXYGEN      =  6.21 KG/HR
BED DIAMETER  = 0.152 METERS            NITROGEN    =  2.72 KG/HR
ESTIMATED BED VOIDAGE = 0.70            PURGE N2    =  5.70 KG/HR
SOLIDS HOLDUP = 6.9 KG                  H2O/CARBON  = 1.72 MOLES H2O/MOLE C
                                        O2/CARBON   = 0.23 MOLES O2/MOLE C
                                        N2/O2       = 0.50 MOLES N2/MOLE O2


                 ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

                     MASS     C        H        O        N        S

          COAL       19.2   10.05     0.80     3.81     0.22    0.152
         GASES       40.6    0.00     2.91    29.28     8.42    0.000
   TOTAL INPUT       59.8   10.05     3.71    33.09     8.64    0.152

          CHAR        3.2    1.31     0.05     0.10     0.03    0.021
          DUST        1.4    0.31     0.06     0.07     0.00    0.003
         GASES       54.5    8.25     3.73    33.72     8.61    0.162
    WASTEWATER        0.0    0.00     0.00     0.00     0.00    0.000
  TOTAL OUTPUT       59.1    9.87     3.83    33.89     8.64    0.186

  % RECOVERY        98.7%   98.3%   103.3%   102.4%   100.1%   122.3%


                       OUTPUT VARIABLES

           CARBON CONVERSION (PERCENT)                82.1
           DRY MAKE GAS FLOW RATE (SCMM)              0.55
           HEATING VALUE OF SWEET GAS (KJ/SCM)       13979
           EFFLUENT FLOW RATES (KG/HR)
                     CO                               7.46
                     H2                               0.96
                     CH4                              1.49
                     CO2                             14.42
                     N2                               8.61
                     H2S                              0.168
                     COS                              0.007
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                    NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                   FLUIDIZED BED COAL GASIFICATION REACTOR

                       RUN GO-73B  3-12-81  11:00-12:00

  REACTOR SPECIFICATIONS                   FEED RATES AND RATIOS

PRESSURE      = 107.1 PSIG             COAL         = 40.25 LB/HR
TEMPERATURE   = 1793.3 DEG.F           STEAM        = 57.27 LB/HR
BED HEIGHT    = 38.0 IN.               OXYGEN       = 14.49 LB/HR
BED DIAMETER  =  6.0 IN.               NITROGEN     =  5.57 LB/HR
ESTIMATED BED VOIDAGE = 0.71           PURGE N2     = 13.32 LB/HR
SOLIDS HOLDUP = 14.9 LB                H2O/CARBON   = 1.90 MOLES H2O/MOLE C
                                       O2/CARBON    = 0.27 MOLES O2/MOLE C
                                       N2/O2        = 0.44 MOLES N2/MOLE O2

                ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                    MASS      C       H       O       N       S

          COAL      40.3    20.09    1.67    8.05    0.40    0.327
         GASES      90.6     0.00    6.41   65.34   18.89    0.000
   TOTAL INPUT     130.9    20.09    8.08   73.39   19.29    0.327

          CHAR       5.0     1.51    0.05    0.26    0.03    0.029
          DUST       1.7     0.48    0.01    0.07    0.01    0.004
         GASES     121.3    17.96    8.30   75.66   19.23    0.150
    WASTEWATER       0.0     0.00    0.00    0.00    0.00    0.000
  TOTAL OUTPUT     128.0    19.94    8.35   75.99   19.27    0.183

  % RECOVERY       97.8%    99.3%  103.4%  103.5%   99.9%    56.0%


                         OUTPUT VARIABLES

          CARBON CONVERSION (PERCENT)               89.4
          DRY MAKE GAS FLOW RATE (SCFM)             19.6
          HEATING VALUE OF SWEET GAS (BTU/SCF)     370.0
          EFFLUENT FLOW RATES (LB/HR)
                      CO                           16.15
                      H2                            2.17
                      CH4                           2.89
                      CO2                          32.50
                      N2                           19.23
                      H2S                           0.153
                      COS                           0.012
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                 NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                 FLUIDIZED BED COAL GASIFICATION REACTOR

                     RUN GO-73B  3-12-81  11:00-12:00

   REACTOR SPECIFICATIONS                 FEED RATES AND RATIOS

 PRESSURE     = 839.4 KPA             COAL        = 18.26 KG/HR
 TEMPERATURE  =  978.5 DEG.C          STEAM       = 25.98 KG/HR
 BED HEIGHT   = 0.97 METERS           OXYGEN      =  6.57 KG/HR
 BED DIAMETER = 0.152 METERS          NITROGEN    =  2.53 KG/HR
 ESTIMATED BED VOIDAGE = 0.71         PURGE N2    =  6.04 KG/HR
 SOLIDS HOLDUP = 6.7 KG               H2O/CARBON = 1.90 MOLES H2O/MOLE C
                                      O2/CARBON  = 0.27 MOLES O2/MOLE C
                                      N2/O2       = 0.44 MOLES N2/MOLE O2

                 ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

                     MASS      C        H        O        N        S

           COAL      18.3     9.11     0.76     3.65     0.18    0.148
           GASES     41.1     0.00     2.91    29.64     8.57    0.000
     TOTAL INPUT     59.4     9.11     3.66    33.29     8.75    0.148

           CHAR       2.3     0.68     0.02     0.12     0.01    0.013
           DUST       0.8     0.22     0.00     0.03     0.00    0.002
           GASES     55.0     8.14     3.76    34.32     8.72    0.068
      WASTEWATER      0.0     0.00     0.00     0.00     0.00    0.000
    TOTAL OUTPUT     58.1     9.05     3.79    34.47     8.74    0.083

    % RECOVERY      97.8%    99.3%   103.4%   103.5%    99.9%    56.0%


                      OUTPUT VARIABLES

           CARBON CONVERSION (PERCENT)               89.4
           DRY MAKE GAS FLOW RATE (SCMM)             0.55
           HEATING VALUE OF SWEET GAS (KJ/SCM)      13785
           EFFLUENT FLOW RATES (KG/HR)
                     CO                              7.32
                     H2                              0.99
                     CH4                             1.31
                     CO2                            14.74
                     N2                              8.72
                     H2S                             0.069
                     COS                             0.006
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NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-74 3-25-81 11:00-12:00

REACTOR SPECIFICATIONS

PRESSURE = 105.5 PSIG
TEMPERATURE = 1658.9 DEG.F
BED HEIGHT = 38.0 IN.
BED DIAMETER = 6.0 IN.
ESTIMATED BED VOIDAGE = 0.80
SOLIDS HOLDUP = 10.4 LB

FEED RATES AND RATIOS

COAL = 67.16 LB/HR
STEAM = 48.57 LB/HR
OXYGEN = 9.25 LB/HR
NITROGEN = 5.66 LB/HR
PURGE N2 = 13.23 LB/HR
H2O/CARBON = 0.97 MOLES H2O/MOLE C
O2/CARBON = 0.10 MOLES O2/MOLE C
N2/O2 = 0.70 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

	MASS	C	H	O	N	S
COAL	67.2	33.52	2.79	13.43	0.67	0.546
GASES	76.7	0.00	5.43	52.38	18.89	0.000
TOTAL INPUT	143.9	33.52	8.22	65.81	19.56	0.546
CHAR	32.0	15.97	0.40	2.71	0.16	0.160
DUST	3.1	0.89	0.02	0.13	0.02	0.007
GASES	102.0	13.32	7.18	61.89	19.38	0.178
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	137.1	30.17	7.60	64.72	19.56	0.345
% RECOVERY	95.3%	90.0%	92.4%	98.4%	100.0%	63.2%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	39.7
DRY MAKE GAS FLOW RATE (SCFM)	15.8
HEATING VALUE OF SWEET GAS (BTU/SCF)	376.8
EFFLUENT FLOW RATES (LB/HR)	
CO	9.87
H2	1.68
CH4	2.89
CO2	25.34
N2	19.38
H2S	0.184
COS	0.009

NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-74 3-25-81 11:00-12:00

REACTOR SPECIFICATIONS

PRESSURE = 828.4 KPA
TEMPERATURE = 903.8 DEG.C
BED HEIGHT = 0.97 METERS
BED DIAMETER = 0.152 METERS
ESTIMATED BED VOIDAGE = 0.80
SOLIDS HOLDUP = 4.7 KG

FEED RATES AND RATIOS

COAL = 30.46 KG/HR
STEAM = 22.03 KG/HR
OXYGEN = 4.19 KG/HR
NITROGEN = 2.57 KG/HR
PURGE N2 = 6.00 KG/HR
H2O/CARBON = 0.97 MOLES H2O/MOLE C
O2/CARBON = 0.10 MOLES O2/MOLE C
N2/O2 = 0.70 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

	MASS	C	H	O	N	S
COAL	30.5	15.20	1.27	6.09	0.30	0.248
GASES	34.8	0.00	2.46	23.76	8.57	0.000
TOTAL INPUT	65.3	15.20	3.73	29.85	8.87	0.248
CHAR	14.5	7.24	0.18	1.23	0.07	0.073
DUST	1.4	0.40	0.01	0.06	0.01	0.003
GASES	46.2	6.04	3.26	28.07	8.79	0.081
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	62.2	13.68	3.45	29.36	8.87	0.156
% RECOVERY	95.3%	90.0%	92.4%	98.4%	100.0%	63.2%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	39.7
DRY MAKE GAS FLOW RATE (SCMM)	0.45
HEATING VALUE OF SWEET GAS (KJ/SCM)	14038
EFFLUENT FLOW RATES (KG/HR)	
CO	4.48
H2	0.76
CH4	1.31
CO2	11.49
N2	8.79
H2S	0.084
COS	0.004

NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-76 4-28-81 13:30-16:15

REACTOR SPECIFICATIONS

PRESSURE = 100.6 PSIG
TEMPERATURE = 1711.6 DEG.F
BED HEIGHT = 38.0 IN.
BED DIAMETER = 6.0 IN.
ESTIMATED BED VOIDAGE = 0.80
SOLIDS HOLDUP = 10.4 LB

FEED RATES AND RATIOS

COAL = 50.86 LB/HR
STEAM = 57.37 LB/HR
OXYGEN = 12.62 LB/HR
NITROGEN = 6.74 LB/HR
PURGE N2 = 10.33 LB/HR
H2O/CARBON = 1.54 MOLES H2O/MOLE C
O2/CARBON = 0.19 MOLES O2/MOLE C
N2/O2 = 0.61 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

	MASS	C	H	O	N	S
COAL	50.9	24.81	1.75	12.89	0.51	0.422
GASES	87.1	0.00	6.42	63.56	17.07	0.000
TOTAL INPUT	137.9	24.81	8.17	76.44	17.58	0.422
CHAR	13.3	6.10	0.12	0.00	0.07	0.077
DUST	0.1	0.03	0.00	0.00	0.00	0.000
GASES	121.6	18.38	8.44	76.97	17.52	0.263
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	135.0	24.51	8.56	76.97	17.59	0.341
% RECOVERY	97.9%	98.8%	104.8%	100.7%	100.0%	80.8%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	74.1
DRY MAKE GAS FLOW RATE (SCFM)	19.2
HEATING VALUE OF SWEET GAS (BTU/SCF)	373.7
EFFLUENT FLOW RATES (LB/HR)	
CO	15.65
H2	2.06
CH4	3.40
CO2	33.42
N2	17.52
H2S	0.271
COS	0.015

NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-76 4-28-81 13:30-16:15

REACTOR SPECIFICATIONS

PRESSURE = 794.9 KPA
TEMPERATURE = 933.1 DEG.C
BED HEIGHT = 0.97 METERS
BED DIAMETER = 0.152 METERS
ESTIMATED BED VOIDAGE = 0.80
SOLIDS HOLDUP = 4.7 KG

FEED RATES AND RATIOS

COAL = 23.07 KG/HR
STEAM = 26.02 KG/HR
OXYGEN = 5.72 KG/HR
NITROGEN = 3.06 KG/HR
PURGE N2 = 4.69 KG/HR
H2O/CARBON = 1.54 MOLES H2O/MOLE C
O2/CARBON = 0.19 MOLES O2/MOLE C
N2/O2 = 0.61 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

	MASS	C	H	O	N	S
COAL	23.1	11.25	0.79	5.84	0.23	0.191
GASES	39.5	0.00	2.91	28.83	7.74	0.000
TOTAL INPUT	62.6	11.25	3.71	34.67	7.98	0.191
CHAR	6.0	2.77	0.06	0.00	0.03	0.035
DUST	0.1	0.01	0.00	0.00	0.00	0.000
GASES	55.1	8.34	3.83	34.91	7.95	0.119
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	61.2	11.12	3.88	34.91	7.98	0.154
% RECOVERY	97.9%	98.8%	104.8%	100.7%	100.0%	80.8%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	74.1
DRY MAKE GAS FLOW RATE (SCMM)	0.54
HEATING VALUE OF SWEET GAS (KJ/SCM)	13922
EFFLUENT FLOW RATES (KG/HR)	
CO	7.10
H2	0.94
CH4	1.54
CO2	15.16
N2	7.95
H2S	0.123
COS	0.007

```
               NCSU DEPARTMENT OF CHEMICAL ENGINEERING

               FLUIDIZED BED COAL GASIFICATION REACTOR

                   RUN GO-78  5-20-81  11:00-12:00

   REACTOR SPECIFICATIONS                FEED RATES AND RATIOS

 PRESSURE     = 103.9 PSIG             COAL       = 41.06 LB/HR
 TEMPERATURE  = 1605.9 DEG.F           STEAM      = 57.35 LB/HR
 BED HEIGHT   = 38.0 IN.               OXYGEN     =  9.14 LB/HR
 BED DIAMETER =  6.0 IN.               NITROGEN   =  6.88 LB/HR
 ESTIMATED BED VOIDAGE = 0.79          PURGE N2   = 15.14 LB/HR
 SOLIDS HOLDUP = 10.9 LB               H2O/CARBON = 1.71 MOLES H2O/MOLE C
                                       O2/CARBON  = 0.15 MOLES O2/MOLE C
                                       N2/O2      = 0.86 MOLES N2/MOLE O2

               ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                   MASS      C        H        O        N        S

          COAL     41.1    22.30     1.90     8.41     0.20    0.319
          GASES    88.5     0.00     6.42    60.07    22.02    0.000
    TOTAL INPUT   129.6    22.30     8.31    68.48    22.22    0.319

          CHAR     13.2     4.96     0.12     0.31     0.07    0.044
          DUST      3.7     1.68     0.04     0.34     0.02    0.016
          GASES   110.5    13.70     7.69    66.71    22.13    0.213
     WASTEWATER     0.0     0.00     0.00     0.00     0.00    0.000
   TOTAL OUTPUT   127.4    20.34     7.86    67.37    22.21    0.274

   % RECOVERY     98.3%    91.2%    94.5%    98.4%   100.0%    85.9%


                       OUTPUT VARIABLES

          CARBON CONVERSION (PERCENT)               61.5
          DRY MAKE GAS FLOW RATE (SCFM)             15.9
          HEATING VALUE OF SWEET GAS (BTU/SCF)     393.4
          EFFLUENT FLOW RATES (LB/HR)
                    CO                               8.73
                    H2                               1.44
                    CH4                              3.60
                    CO2                             26.61
                    N2                              22.13
                    H2S                              0.220
                    COS                              0.012
```

NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-78 5-20-81 11:00-12:00

REACTOR SPECIFICATIONS

PRESSURE = 817.5 KPA
TEMPERATURE = 874.4 DEG.C
BED HEIGHT = 0.97 METERS
BED DIAMETER = 0.152 METERS
ESTIMATED BED VOIDAGE = 0.79
SOLIDS HOLDUP = 4.9 KG

FEED RATES AND RATIOS

COAL = 18.62 KG/HR
STEAM = 26.01 KG/HR
OXYGEN = 4.15 KG/HR
NITROGEN = 3.12 KG/HR
PURGE N2 = 6.87 KG/HR
H2O/CARBON = 1.71 MOLES H2O/MOLE C
O2/CARBON = 0.15 MOLES O2/MOLE C
N2/O2 = 0.86 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

	MASS	C	H	O	N	S
COAL	18.6	10.11	0.86	3.82	0.09	0.145
GASES	40.1	0.00	2.91	27.25	9.99	0.000
TOTAL INPUT	58.8	10.11	3.77	31.06	10.08	0.145
CHAR	6.0	2.25	0.06	0.14	0.03	0.020
DUST	1.7	0.76	0.02	0.16	0.01	0.007
GASES	50.1	6.22	3.49	30.26	10.04	0.097
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	57.8	9.23	3.56	30.56	10.08	0.124
% RECOVERY	98.3%	91.2%	94.5%	98.4%	100.0%	85.9%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	61.5
DRY MAKE GAS FLOW RATE (SCMM)	0.45
HEATING VALUE OF SWEET GAS (KJ/SCM)	14657
EFFLUENT FLOW RATES (KG/HR)	
CO	3.96
H2	0.65
CH4	1.63
CO2	12.07
N2	10.04
H2S	0.100
COS	0.005

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                 NCSU DEPARTMENT OF CHEMICAL ENGINEERING

                 FLUIDIZED BED COAL GASIFICATION REACTOR


                     RUN GO-79  6-10-81  11:00-11:40


   REACTOR SPECIFICATIONS              FEED RATES AND RATIOS

 PRESSURE     = 103.5 PSIG          COAL       = 36.00 LB/HR
 TEMPERATURE  = 1747.6 DEG.F        STEAM      = 57.35 LB/HR
 BED HEIGHT   = 38.0 IN.            OXYGEN     = 11.87 LB/HR
 BED DIAMETER =  6.0 IN.            NITROGEN   =  7.96 LB/HR
 ESTIMATED BED VOIDAGE = 0.83       PURGE N2   = 11.84 LB/HR
 SOLIDS HOLDUP =  8.5 LB            H2O/CARBON = 2.03 MOLES H2O/MOLE C
                                    O2/CARBON  = 0.24 MOLES O2/MOLE C
                                    N2/O2      = 0.77 MOLES N2/MOLE O2


                 ELEMENTAL MATERIAL BALANCES : FLOWS IN LB/HR

                     MASS      C       H        O        N       S

          COAL       36.0    18.85    1.64     6.90     0.40   0.307
         GASES       89.0     0.00    6.42    62.79    19.80   0.000
   TOTAL INPUT      125.0    18.85    8.06    69.69    20.20   0.307

          CHAR        5.4     0.45    0.02     0.77     0.01   0.029
          DUST        1.1     0.38    0.01     0.04     0.01   0.003
         GASES      119.5    16.92    8.33    73.84    20.16   0.214
    WASTEWATER        0.0     0.00    0.00     0.00     0.00   0.000
  TOTAL OUTPUT      126.0    17.75    8.36    74.65    20.19   0.246

  % RECOVERY     100.8%    94.2%  103.7%   107.1%    99.9%   80.2%


                        OUTPUT VARIABLES

            CARBON CONVERSION (PERCENT)               89.8
            DRY MAKE GAS FLOW RATE (SCFM)             18.7
            HEATING VALUE OF SWEET GAS (BTU/SCF)     364.7
            EFFLUENT FLOW RATES (LB/HR)
                      CO                             15.06
                      H2                              1.97
                      CH4                             3.28
                      CO2                            29.34
                      N2                             20.16
                      H2S                             0.218
                      COS                             0.016
```

NCSU DEPARTMENT OF CHEMICAL ENGINEERING

FLUIDIZED BED COAL GASIFICATION REACTOR

RUN GO-79 6-10-81 11:00-11:40

REACTOR SPECIFICATIONS

PRESSURE = 815.0 KPA
TEMPERATURE = 953.1 DEG.C
BED HEIGHT = 0.97 METERS
BED DIAMETER = 0.152 METERS
ESTIMATED BED VOIDAGE = 0.83
SOLIDS HOLDUP = 3.8 KG

FEED RATES AND RATIOS

COAL = 16.33 KG/HR
STEAM = 26.01 KG/HR
OXYGEN = 5.38 KG/HR
NITROGEN = 3.61 KG/HR
PURGE N2 = 5.37 KG/HR
H2O/CARBON = 2.03 MOLES H2O/MOLE C
O2/CARBON = 0.24 MOLES O2/MOLE C
N2/O2 = 0.77 MOLES N2/MOLE O2

ELEMENTAL MATERIAL BALANCES : FLOWS IN KG/HR

	MASS	C	H	O	N	S
COAL	16.3	8.55	0.75	3.13	0.18	0.139
GASES	40.4	0.00	2.91	28.48	8.98	0.000
TOTAL INPUT	56.7	8.55	3.66	31.61	9.16	0.139
CHAR	2.4	0.21	0.01	0.35	0.01	0.013
DUST	0.5	0.17	0.00	0.02	0.00	0.002
GASES	54.2	7.68	3.78	33.49	9.15	0.097
WASTEWATER	0.0	0.00	0.00	0.00	0.00	0.000
TOTAL OUTPUT	57.1	8.05	3.79	33.86	9.16	0.112
% RECOVERY	100.8%	94.2%	103.7%	107.1%	99.9%	80.2%

OUTPUT VARIABLES

CARBON CONVERSION (PERCENT)	89.8
DRY MAKE GAS FLOW RATE (SCMM)	0.53
HEATING VALUE OF SWEET GAS (KJ/SCM)	13586
EFFLUENT FLOW RATES (KG/HR)	
CO	6.83
H2	0.89
CH4	1.49
CO2	13.31
N2	9.15
H2S	0.099
COS	0.007

APPENDIX B
GASIFIER MODEL RESULTS

WELL-MIXED COAL GASIFICATION MODEL RESULTS

GO-66 10-22-80 11:30-13:00

REACTOR SPECIFICATIONS	
BED PRESSURE(PSIG)	103.60
BED TEMPERATURE(F)	1798.50
SOLIDS HOLDUP(LB)	13.50
BED HEIGHT(IN)	38.00
BED DIAMETER(IN)	6.00
BED VOIDAGE	0.81

MODEL PARAMETERS	
CHAR REACTIVITY	0.2170
COMBUSTION EXTENT	0.5040
SHIFT REACTIVITY	3.660E-04

FEEDRATES (LB/HR)	
INLET COAL	42.64
STEAM	57.30
OXYGEN	17.80
NITROGEN	5.29
HYDROGEN	0.00
PURGE N2	9.06

FEED COAL ANALYSIS (WT %)	
CARBON	53.00
HYDROGEN	4.70
OXYGEN	18.30
NITROGEN	0.50
SULFUR	0.80
ASH	22.70

	MODEL	EXPERIMENTAL
DRY GAS FLOW RATE (SCFM)	20.20	19.79
CARBON CONVERSION		
DEVOLATILIZATION	0.229	
COMBUSTION	0.587	
GASIFICATION	0.092	
TOTAL	0.908	0.968
SWEET GAS HEATING VALUE (BTU/SCF)	378.4	407.1

GAS COMPOSITION (MOLE PERCENT)

	MODEL	EXPERIMENTAL
CO	11.16	11.28
H2	19.32	15.98
CH4	4.23	4.77
CO2	13.56	14.80
N2	8.80	8.80
H2S	0.16	0.18
COS	0.01	0.01
H2O	42.78	44.20

WELL-MIXED COAL GASIFICATION MODEL RESULTS

GO-68B 11-19-80 14:00-16:30

REACTOR SPECIFICATIONS

BED PRESSURE(PSIG)	105.00
BED TEMPERATURE(F)	1786.50
SOLIDS HOLDUP(LB)	10.40
BED HEIGHT(IN)	38.00
BED DIAMETER(IN)	6.00
BED VOIDAGE	0.85

FEEDRATES (LB/HR)

INLET COAL	63.60
STEAM	56.83
OXYGEN	17.64
NITROGEN	6.27
HYDROGEN	0.00
PURGE N2	13.36

MODEL PARAMETERS

CHAR REACTIVITY	0.2170
COMBUSTION EXTENT	0.5040
SHIFT REACTIVITY	3.660E-04

FEED COAL ANALYSIS (WT %)

CARBON	53.00
HYDROGEN	4.70
OXYGEN	18.30
NITROGEN	0.50
SULFUR	0.80
ASH	22.70

	MODEL	EXPERIMENTAL
DRY GAS FLOW RATE (SCFM)	23.82	23.35
CARBON CONVERSION		
DEVOLATILIZATION	0.227	
COMBUSTION	0.390	
GASIFICATION	0.079	
TOTAL	0.696	0.669
SWEET GAS HEATING VALUE (BTU/SCF)	394.3	381.1

GAS COMPOSITION (MOLE PERCENT)

	MODEL	EXPERIMENTAL
CO	11.62	12.66
H2	19.99	20.00
CH4	5.59	4.06
CO2	12.64	12.54
N2	10.80	11.05
H2S	0.15	0.15
COS	0.01	0.01
H2O	39.20	39.49

WELL-MIXED COAL GASIFICATION MODEL RESULTS

GO-69B 12-15-80 13:30-16:00

REACTOR SPECIFICATIONS		FEEDRATES (LB/HR)	
BED PRESSURE(PSIG)	105.80	INLET COAL	54.83
BED TEMPERATURE(F)	1720.20	STEAM	56.71
SOLIDS HOLDUP(LB)	8.40	OXYGEN	15.50
BED HEIGHT(IN)	38.00	NITROGEN	8.19
BED DIAMETER(IN)	6.00	HYDROGEN	0.00
BED VOIDAGE	0.88	PURGE N2	12.18

MODEL PARAMETERS		FEED COAL ANALYSIS (WT %)	
CHAR REACTIVITY	0.2170	CARBON	44.20
COMBUSTION EXTENT	0.5040	HYDROGEN	3.70
SHIFT REACTIVITY	3.660E-04	OXYGEN	18.30
		NITROGEN	0.50
		SULFUR	0.80
		ASH	32.60

	MODEL	EXPERIMENTAL
DRY GAS FLOW RATE (SCFM)	19.52	19.25
CARBON CONVERSION		
DEVOLATILIZATION	0.218	
COMBUSTION	0.476	
GASIFICATION	0.062	
TOTAL	0.756	0.680
SWEET GAS HEATING VALUE (BTU/SCF)	360.7	377.6

GAS COMPOSITION (MOLE PERCENT)

	MODEL	EXPERIMENTAL
CO	8.87	6.93
H2	16.80	17.99
CH4	3.97	3.74
CO2	12.78	11.99
N2	12.35	12.11
H2S	0.15	0.15
COS	0.00	0.00
H2O	45.06	47.08

WELL-MIXED COAL GASIFICATION MODEL RESULTS

GO-70 1-8-81 14:00-16:30

REACTOR SPECIFICATIONS

BED PRESSURE(PSIG)	105.80
BED TEMPERATURE(F)	1781.10
SOLIDS HOLDUP(LB)	10.00
BED HEIGHT(IN)	38.00
BED DIAMETER(IN)	6.00
BED VOIDAGE	0.85

FEEDRATES (LB/HR)

INLET COAL	48.38
STEAM	57.61
OXYGEN	16.79
NITROGEN	5.62
HYDROGEN	0.00
PURGE N2	13.42

MODEL PARAMETERS

CHAR REACTIVITY	0.2170
COMBUSTION EXTENT	0.5040
SHIFT REACTIVITY	3.660E-04

FEED COAL ANALYSIS (WT %)

CARBON	43.90
HYDROGEN	3.70
OXYGEN	19.20
NITROGEN	0.50
SULFUR	0.80
ASH	32.00

	MODEL	EXPERIMENTAL
DRY GAS FLOW RATE (SCFM)	19.75	20.20
CARBON CONVERSION		
DEVOLATILIZATION	0.220	
COMBUSTION	0.589	
GASIFICATION	0.090	
TOTAL	0.898	0.862
SWEET GAS HEATING VALUE (BTU/SCF)	367.7	379.4

GAS COMPOSITION (MOLE PERCENT)

	MODEL	EXPERIMENTAL
CO	9.83	9.60
H2	17.14	19.18
CH4	3.48	3.73
CO2	13.36	12.32
N2	11.55	11.57
H2S	0.16	0.14
COS	0.01	0.00
H2O	44.47	43.43

WELL-MIXED COAL GASIFICATION MODEL RESULTS

GO-71B 1-27-81 14:30-15:30

REACTOR SPECIFICATIONS	
BED PRESSURE(PSIG)	105.20
BED TEMPERATURE(F)	1798.40
SOLIDS HOLDUP(LB)	12.30
BED HEIGHT(IN)	38.00
BED DIAMETER(IN)	6.00
BED VOIDAGE	0.82

FEEDRATES (LB/HR)	
INLET COAL	45.81
STEAM	57.28
OXYGEN	16.04
NITROGEN	5.80
HYDROGEN	0.00
PURGE N2	11.45

MODEL PARAMETERS	
CHAR REACTIVITY	0.2170
COMBUSTION EXTENT	0.5040
SHIFT REACTIVITY	3.660E-04

FEED COAL ANALYSIS (WT %)	
CARBON	50.60
HYDROGEN	4.20
OXYGEN	20.40
NITROGEN	1.00
SULFUR	0.80
ASH	23.00

	MODEL	EXPERIMENTAL
DRY GAS FLOW RATE (SCFM)	20.36	21.65
CARBON CONVERSION		
DEVOLATILIZATION	0.227	
COMBUSTION	0.515	
GASIFICATION	0.121	
TOTAL	0.863	0.891
SWEET GAS HEATING VALUE (BTU/SCF)	373.6	385.4

GAS COMPOSITION (MOLE PERCENT)

	MODEL	EXPERIMENTAL
CO	10.70	11.13
H2	18.50	20.15
CH4	4.09	4.08
CO2	13.25	12.70
N2	10.58	10.22
H2S	0.15	0.21
COS	0.01	0.01
H2O	42.73	41.51

```
                 WELL-MIXED COAL GASIFICATION MODEL RESULTS

                        GO-72  2-19-81  12:30-14:30

    REACTOR SPECIFICATIONS                     FEEDRATES (LB/HR)

    BED PRESSURE(PSIG)      104.40             INLET COAL             42.33
    BED TEMPERATURE(F)     1797.30             STEAM                  57.29
    SOLIDS HOLDUP(LB)        15.10             OXYGEN                 13.69
    BED HEIGHT(IN)           38.00             NITROGEN                5.99
    BED DIAMETER(IN)          6.00             HYDROGEN                0.00
    BED VOIDAGE               0.78             PURGE N2               12.67


    MODEL PARAMETERS                           FEED COAL ANALYSIS (WT %)

    CHAR REACTIVITY         0.2170             CARBON                 52.30
    COMBUSTION EXTENT       0.5040             HYDROGEN                4.20
    SHIFT REACTIVITY    3.660E-04              OXYGEN                 17.50
                                               NITROGEN                1.00
                                               SULFUR                  0.80
                                               ASH                    24.20


                                            MODEL    EXPERIMENTAL

            DRY GAS FLOW RATE (SCFM)        19.55       19.49

            CARBON CONVERSION
              DEVOLATILIZATION              0.216
              COMBUSTION                    0.460
              GASIFICATION                  0.140
              TOTAL                         0.817       0.821

            SWEET GAS HEATING
              VALUE (BTU/SCF)               370.8       375.9


                      GAS COMPOSITION (MOLE PERCENT)

                                MODEL    EXPERIMENTAL

                      CO         9.80       10.02
                      H2        18.59       17.80
                      CH4        3.99        3.48
                      CO2       12.25       12.33
                      N2        11.72       11.57
                      H2S        0.14        0.19
                      COS        0.00        0.00
                      H2O       43.51       44.60
```

WELL-MIXED COAL GASIFICATION MODEL RESULTS

GO-73B 3-12-81 11:00-12:00

REACTOR SPECIFICATIONS

BED PRESSURE(PSIG)	107.10
BED TEMPERATURE(F)	1793.30
SOLIDS HOLDUP(LB)	14.90
BED HEIGHT(IN)	38.00
BED DIAMETER(IN)	6.00
BED VOIDAGE	0.79

FEEDRATES (LB/HR)

INLET COAL	40.25
STEAM	57.27
OXYGEN	14.49
NITROGEN	5.57
HYDROGEN	0.00
PURGE N2	13.32

MODEL PARAMETERS

CHAR REACTIVITY	0.2170
COMBUSTION EXTENT	0.5040
SHIFT REACTIVITY	3.660E-04

FEED COAL ANALYSIS (WT %)

CARBON	49.90
HYDROGEN	4.20
OXYGEN	17.70
NITROGEN	1.00
SULFUR	0.80
ASH	26.50

	MODEL	EXPERIMENTAL
DRY GAS FLOW RATE (SCFM)	19.13	19.60
CARBON CONVERSION		
DEVOLATILIZATION	0.229	
COMBUSTION	0.537	
GASIFICATION	0.119	
TOTAL	0.886	0.894
SWEET GAS HEATING VALUE (BTU/SCF)	371.2	370.0

GAS COMPOSITION (MOLE PERCENT)

	MODEL	EXPERIMENTAL
CO	9.35	9.71
H2	17.84	18.13
CH4	3.81	3.03
CO2	12.57	12.44
N2	11.95	11.56
H2S	0.14	0.08
COS	0.00	0.00
H2O	44.33	45.05

WELL-MIXED COAL GASIFICATION MODEL RESULTS

GO-74 3-25-81 11:00-12:00

REACTOR SPECIFICATIONS	
BED PRESSURE(PSIG)	105.50
BED TEMPERATURE(F)	1658.90
SOLIDS HOLDUP(LB)	10.40
BED HEIGHT(IN)	38.00
BED DIAMETER(IN)	6.00
BED VOIDAGE	0.80

FEEDRATES (LB/HR)	
INLET COAL	67.16
STEAM	48.57
OXYGEN	9.25
NITROGEN	5.66
HYDROGEN	0.00
PURGE N2	13.23

MODEL PARAMETERS	
CHAR REACTIVITY	0.2170
COMBUSTION EXTENT	0.5040
SHIFT REACTIVITY	3.660E-04

FEED COAL ANALYSIS (WT %)	
CARBON	49.90
HYDROGEN	4.20
OXYGEN	17.70
NITROGEN	1.00
SULFUR	0.80
ASH	26.50

	MODEL	EXPERIMENTAL
DRY GAS FLOW RATE (SCFM)	17.22	15.80
CARBON CONVERSION		
DEVOLATILIZATION	0.220	
COMBUSTION	0.206	
GASIFICATION	0.034	
TOTAL	0.460	0.397
SWEET GAS HEATING VALUE (BTU/SCF)	412.9	376.8

GAS COMPOSITION (MOLE PERCENT)

	MODEL	EXPERIMENTAL
CO	7.11	7.04
H2	17.00	16.65
CH4	6.29	3.61
CO2	10.42	11.51
N2	12.70	13.83
H2S	0.11	0.11
COS	0.00	0.00
H2O	46.36	47.25

```
                 WELL-MIXED COAL GASIFICATION MODEL RESULTS

                        GO-76  4-28-81  13:30-16:15

REACTOR SPECIFICATIONS                    FEEDRATES (LB/HR)

BED PRESSURE(PSIG)      100.60            INLET COAL               50.86
BED TEMPERATURE(F)     1711.60            STEAM                    57.37
SOLIDS HOLDUP(LB)        10.40            OXYGEN                   12.62
BED HEIGHT(IN)           38.00            NITROGEN                  6.74
BED DIAMETER(IN)          6.00            HYDROGEN                  0.00
BED VOIDAGE               0.80            PURGE N2                 10.33

MODEL PARAMETERS                          FEED COAL ANALYSIS (WT %)

CHAR REACTIVITY         0.2170            CARBON                   48.80
COMBUSTION EXTENT       0.5040            HYDROGEN                  4.00
SHIFT REACTIVITY    3.660E-04             OXYGEN                   22.70
                                          NITROGEN                  1.00
                                          SULFUR                    0.80
                                          ASH                      22.80

                                          MODEL    EXPERIMENTAL

        DRY GAS FLOW RATE (SCFM)          18.40       19.20

        CARBON CONVERSION
          DEVOLATILIZATION                0.228
          COMBUSTION                      0.379
          GASIFICATION                    0.099
          TOTAL                           0.706       0.741

        SWEET GAS HEATING
          VALUE (BTU/SCF)                 374.8       373.7

                     GAS COMPOSITION (MOLE PERCENT)

                          MODEL    EXPERIMENTAL

                  CO       8.34        9.44
                  H2      17.24       17.25
                  CH4      4.38        3.58
                  CO2     12.54       12.84
                  N2      10.75       10.57
                  H2S      0.13        0.13
                  COS      0.00        0.00
                  H2O     46.63       46.18
```

WELL-MIXED COAL GASIFICATION MODEL RESULTS

GO-78 5-20-81 11:00-12:00

REACTOR SPECIFICATIONS	
BED PRESSURE(PSIG)	103.90
BED TEMPERATURE(F)	1605.90
SOLIDS HOLDUP(LB)	10.90
BED HEIGHT(IN)	38.00
BED DIAMETER(IN)	6.00
BED VOIDAGE	0.79

FEEDRATES (LB/HR)	
INLET COAL	41.06
STEAM	57.35
OXYGEN	9.14
NITROGEN	6.88
HYDROGEN	0.00
PURGE N2	15.14

MODEL PARAMETERS	
CHAR REACTIVITY	0.2170
COMBUSTION EXTENT	0.5040
SHIFT REACTIVITY	3.660E-04

FEED COAL ANALYSIS (WT %)	
CARBON	54.20
HYDROGEN	4.60
OXYGEN	18.60
NITROGEN	0.50
SULFUR	0.80
ASH	21.40

	MODEL	EXPERIMENTAL
DRY GAS FLOW RATE (SCFM)	15.41	15.90
CARBON CONVERSION		
DEVOLATILIZATION	0.213	
COMBUSTION	0.306	
GASIFICATION	0.033	
TOTAL	0.552	0.616
SWEET GAS HEATING VALUE (BTU/SCF)	372.3	393.4

GAS COMPOSITION (MOLE PERCENT)

	MODEL	EXPERIMENTAL
CO	5.02	5.88
H2	13.92	13.43
CH4	3.99	4.24
CO2	9.62	11.41
N2	14.42	14.91
H2S	0.09	0.12
COS	0.00	0.00
H2O	52.93	50.00

```
                    WELL-MIXED COAL GASIFICATION MODEL RESULTS

                          GO-79  6-10-81  11:00-11:40

REACTOR SPECIFICATIONS                     FEEDRATES (LB/HR)

BED PRESSURE(PSIG)      103.50             INLET COAL               36.00
BED TEMPERATURE(F)     1747.60             STEAM                    57.35
SOLIDS HOLDUP(LB)         8.50             OXYGEN                   11.87
BED HEIGHT(IN)           38.00             NITROGEN                  7.96
BED DIAMETER(IN)          6.00             HYDROGEN                  0.00
BED VOIDAGE               0.83             PURGE N2                 12.06


MODEL PARAMETERS                           FEED COAL ANALYSIS (WT %)

CHAR REACTIVITY         0.2170             CARBON                   52.10
COMBUSTION EXTENT       0.5040             HYDROGEN                  4.60
SHIFT REACTIVITY     3.660E-04             OXYGEN                   17.70
                                           NITROGEN                  0.50
                                           SULFUR                    0.90
                                           ASH                      24.30


                                        MODEL    EXPERIMENTAL

        DRY GAS FLOW RATE (SCFM)        17.28       18.70

        CARBON CONVERSION
          DEVOLATILIZATION              0.225
          COMBUSTION                    0.471
          GASIFICATION                  0.097
          TOTAL                         0.794       0.903

        SWEET GAS HEATING
          VALUE (BTU/SCF)               353.8       366.1


                   GAS COMPOSITION (MOLE PERCENT)

                        MODEL    EXPERIMENTAL

                   CO    7.33        9.19
                   H2   16.67       16.64
                   CH4   3.63        3.49
                   CO2  11.34       11.40
                   N2   12.97       12.30
                   H2S   0.13        0.11
                   COS   0.00        0.00
                   H2O  47.92       46.88
```

APPENDIX C
GAS STREAM COMPOSITION DATA
CHAR GASIFICATION RUNS

TABLE C-1
GAS ANALYSIS SUMMARY FOR AMI-30/GO-56

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	33.26	33.26	33.17	43.19	15.24	0.00
CO_2	24.98	24.98	24.60	1.46	43.20	71.50
C_2H_4	-----	-----	-----	-----	-----	-----
C_2H_6	-----	-----	-----	-----	-----	-----
H_2S	0.8294	0.8294	0.910	0.048	0.634	2.539
COS	0.041	0.041	0.042	0.003	0.043	0.117
N_2	18.15	18.15	18.50	24.89	14.75	24.56
CH_4	1.64	1.64	1.64	1.95	3.40	0.42
CO	21.03	21.03	21.06	28.48	22.72	1.02
C_6H_6	-----	-----	-----	-----	-----	-----
C_7H_8	-----	-----	-----	-----	-----	-----
Ethyl Benz.	-----	-----	-----	-----	-----	-----
Xylenes	-----	-----	-----	-----	-----	-----
Thiophene*	-----	-----	-----	-----	-----	-----
CH_3SH*	-----	-----	-----	-----	-----	-----
C_2H_5SH*	-----	-----	-----	-----	-----	-----
CS_2	TRACE	TRACE	TRACE	TRACE	TRACE	TRACE
Propylene*	-----	-----	-----	-----	-----	-----
Propane*	-----	-----	-----	-----	-----	-----
Butane*	-----	-----	-----	-----	-----	-----
Methanol**	-----	-----	-----	-----	-----	1.32

*Parts per Million (volume) **Estimated

TABLE C-2
GAS ANALYSIS SUMMARY FOR AMI-35/GO-59

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	32.77	32.77	33.19	45.50	12.88	0.00
CO_2	27.91	27.91	28.01	0.95	43.81	73.17
C_2H_4	-----	-----	-----	-----	-----	-----
C_2H_6	-----	-----	-----	-----	-----	-----
H_2S	0.8470	0.8470	0.807	0.037	0.526	1.970
COS	0.0306	0.0306	0.045	0.003	0.038	0.127
N_2	16.99	16.99	15.70	23.23	13.92	21.12
CH_4	2.15	2.15	2.01	2.44	4.24	0.70
CO	19.30	19.30	20.20	27.85	24.59	1.66
C_6H_6	-----	-----	-----	-----	-----	-----
C_7H_8	-----	-----	-----	-----	-----	-----
Ethyl Benz.	-----	-----	-----	-----	-----	-----
Xylenes	-----	-----	-----	-----	-----	-----
Thiophene*	-----	-----	-----	-----	-----	-----
CH_3SH*	-----	-----	-----	-----	-----	-----
C_2H_5SH*	-----	-----	-----	-----	-----	-----
CS_2	TRACE	TRACE	TRACE	TRACE	TRACE	TRACE
Propylene*	-----	-----	-----	-----	-----	-----
Propane*	-----	-----	-----	-----	-----	-----
Butane*	-----	-----	-----	-----	-----	-----
Methanol**	-----	-----	-----	-----	-----	1.20

*Parts per Million (volume) **Estimated

TABLE C-3
GAS ANALYSIS SUMMARY FOR AMI-36/GO-60

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	31.58	31.58	33.44	44.31	13.87	0.00
CO_2	20.08	20.08	20.90	0.42	34.17	70.53
C_2H_4	-----	-----	-----	-----	-----	-----
C_2H_6	-----	-----	-----	-----	-----	-----
H_2S	0.8887	0.8887	0.892	0.068	0.569	2.539
COS	0.0332	0.0332	0.048	0.004	0.038	0.117
N_2	30.04	30.04	26.19	33.04	26.49	23.58
CH_4	1.28	1.28	1.27	1.68	2.83	0.40
CO	16.11	16.11	17.03	20.58	22.02	0.98
C_6H_6	-----	-----	-----	-----	-----	-----
C_7H_8	-----	-----	-----	-----	-----	-----
Ethyl Benz.	-----	-----	-----	-----	-----	-----
Xylenes	-----	-----	-----	-----	-----	-----
Thiophene*	-----	-----	-----	-----	-----	-----
CH_3SH*	-----	-----	-----	-----	-----	-----
C_2H_5SH*	-----	-----	-----	-----	-----	-----
CS_2*	TRACE	TRACE	TRACE	TRACE	TRACE	TRACE
Propylene*	-----	-----	-----	-----	-----	-----
Propane*	-----	-----	-----	-----	-----	-----
Butane*	-----	-----	-----	-----	-----	-----
Methanol**	-----	-----	-----	-----	-----	1.32

*Parts per Million (volume) **Estimated

TABLE C-4
GAS ANALYSIS SUMMARY FOR AMI-37/GO-61

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	35.35	35.35	38.93	54.96	11.88	0.00
CO_2	24.39	24.39	25.05	0.64	47.82	72.90
C_2H_4	-----	-----	-----	-----	-----	-----
C_2H_6	-----	-----	-----	-----	-----	-----
H_2S	0.8611	0.8611	0.863	0.041	0.628	2.260
COS	0.0333	0.0333	0.047	0.003	0.043	0.130
N_2	20.67	20.67	14.82	19.30	12.94	21.70
CH_4	1.15	1.15	1.15	1.16	3.14	0.23
CO	17.55	17.55	18.81	23.92	22.34	0.96
C_6H_6	-----	-----	-----	-----	-----	-----
C_7H_8	-----	-----	-----	-----	-----	-----
Ethyl Benz.	-----	-----	-----	-----	-----	-----
Xylenes	-----	-----	-----	-----	-----	-----
Thiophene*	-----	-----	-----	-----	-----	-----
CH_3SH*	-----	-----	-----	-----	-----	-----
C_2H_5SH*	-----	-----	-----	-----	-----	-----
CS_2	TRACE	TRACE	TRACE	TRACE	TRACE	TRACE
Propylene*	-----	-----	-----	-----	-----	-----
Propane*	-----	-----	-----	-----	-----	-----
Butane*	-----	-----	-----	-----	-----	-----
Methanol**	-----	-----	-----	-----	-----	1.53

*Parts per Million (volume) **Estimated

APPENDIX D
GAS STREAM COMPOSITION DATA
COAL GASIFICATION RUNS

TABLE D-1
GAS ANALYSIS SUMMARIES FOR GO-66 AND GO-74

	GO-66		GO-74	
Species	Sample Train	PCS Tank	Sample Train	PCS Tank
H_2	28.39	29.02	31.05	30.94
CO_2	26.30	26.37	21.46	21.53
C_2H_4	0.25	0.28	0.46	0.30
C_2H_6	0.36	0.40	0.57	0.40
H_2S	0.315	0.268	0.205	0.195
COS	0.0120	0.0100	0.0059	0.0056
N_2	15.64	15.01	25.78	26.16
CH_4	8.47	8.27	6.72	6.93
CO	20.05	20.17	13.13	13.14
C_6H_6	0.1066	0.1062	0.0886	0.0920
C_7H_8	0.0872	0.0888	0.1177	0.1173
Ethyl Benz.	N/A	N/A	N/A	N/A
Xylenes	N/A	N/A	N/A	N/A
Thiophene*	N/A	N/A	22	24
CH_3SH*	6	5	15	-----
C_2H_5SH*	-----	-----	-----	-----
CS_2*	2	2	1	1
Propylene*	N/A	N/A	2711	1014
Propane*	N/A	N/A	868	476
Butane*	N/A	N/A	351	187

*Parts per million (volume)

TABLE D-2
GAS ANALYSIS SUMMARY FOR AMI-43/GO-68B

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	32.71	32.80	32.57	43.40	9.39	0.00
CO_2	20.46	20.37	20.15	-----	50.58	68.37
C_2H_4	0.388	0.398	0.310	0.062	2.054	0.313
C_2H_6	0.602	0.621	0.511	0.112	3.083	0.446
H_2S	0.254	0.242	0.295	0.022	0.254	0.568
COS	0.0117	0.0106	0.0119	0.0012	0.0153	0.0315
N_2	18.49	17.75	18.79	23.01	9.08	28.21
CH_4	6.43	6.67	6.62	7.53	10.64	0.52
CO	21.16	20.90	21.23	25.79	14.81	0.08
C_6H_6	N/A	N/A	N/A	N/A	N/A	N/A
C_7H_8	N/A	N/A	N/A	N/A	N/A	N/A
Ethyl Benz.	N/A	N/A	N/A	N/A	N/A	N/A
Xylenes	N/A	N/A	N/A	N/A	N/A	N/A
Thiophene*	23	23	22	17	16	18
CH_3SH*	22	18	26	1	3	11
C_2H_5SH*	-----	1	1	-----	-----	1
CS_2*	2	2	2	1	1	3
Propylene*	1113	1567	880	-----	2597	1120
Propane*	183	361	147	-----	288	247
Butane*	N/A	N/A	N/A	N/A	N/A	N/A
Methanol**	-----	-----	-----	-----	-----	1.10

*Parts per million (volume) **Estimated

TABLE D-3
GAS ANALYSIS SUMMARY FOR AMI-44/GO-69B

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	29.97	30.23	30.47	39.45	18.33	0.78
CO_2	22.27	22.83	22.20	1.29	34.28	62.41
C_2H_4	0.42	0.42	0.43	0.26	0.71	0.69
C_2H_6	0.48	0.48	0.49	0.33	0.79	0.73
H_2S	0.26	0.29	0.29	0.028	0.18	0.70
COS	0.0079	0.0084	0.0112	0.001	0.0084	0.02
N_2	25.20	24.38	24.66	31.89	23.00	25.03
CH_4	7.44	7.14	7.25	8.60	9.25	1.59
CO	13.75	14.24	14.26	18.34	13.64	0.94
C_6H_6	0.087	0.092	0.086	0.0008	0.0026	0.18
C_7H_8	0.028	0.039	0.030	0.0005	0.0029	0.014
Ethyl Benz.	0.00095	0.0027	0.0006	-----	-----	-----
Xylenes	0.0061	0.0175	0.0022	-----	-----	-----
Thiophene*	26	36	19	-----	-----	-----
CH_3SH*	16	18	27	38	1	4
C_2H_5SH*	-----	-----	-----	-----	-----	-----
CS_2*	1	1	1	2	1	1
Propylene*	2050	2034	N/A	393	2015	5923
Propane*	693	643	N/A	529	197	1544
Butane*	N/A	N/A	N/A	N/A	N/A	N/A
Methanol**	-----	-----	-----	-----	-----	1.24

*Parts per million (volume) **Estimated

TABLE D-4
GAS ANALYSIS SUMMARY FOR AMI-45/GO-70

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	31.47	26.41	31.12	40.90	19.31	0.51
CO_2	21.29	18.65	20.72	2.58	12.51	58.02
C_2H_4	0.35	0.29	0.37	0.023	0.39	1.06
C_2H_6	0.52	0.44	0.52	0.037	0.62	1.60
H_2S	0.24	N/A	0.255	0.026	0.100	0.52
COS	0.0076	0.0033	0.0079	0.0005	0.0032	0.023
N_2	22.07	28.18	21.49	27.93	24.11	27.27
CH_4	6.16	5.15	6.03	5.28	13.38	5.04
CO	17.86	15.09	17.54	20.89	25.64	3.43
C_6H_6	0.092	0.092	0.79	0.0004	0.0008	0.0077
C_7H_8	0.021	0.022	0.37	0.0002	0.0004	0.0091
Ethyl Benz.	0.0008	0.0011	0.0094	-----	-----	TRACE
Xylenes	0.0037	0.0062	0.0071	0.0005	-----	0.0001
Thiophene*	26	30	38	-----	-----	TRACE
CH_3SH*	7	8	13	1	2	9
C_2H_5SH*	TRACE	TRACE	5	2	TRACE	TRACE
CS_2*	3	4	36	1	1	2
Propylene*	5482	5269	5447	155	444	1719
Propane*	830	726	950	161	379	282
Butane*	310	286	335	-----	-----	-----
Methanol**	-----	-----	-----	-----	-----	0.43

*Parts per million (volume) **Estimated

TABLE D-5
GAS ANALYSIS SUMMARY FOR AMI-47/GO-71B

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	34.14	33.67	34.04	44.99	17.50	-----
CO_2	21.51	22.00	21.92	0.09	9.30	61.37
C_2H_4	0.33	0.29	0.32	-----	0.32	0.96
C_2H_6	0.55	0.51	0.58	-----	0.61	1.67
H_2S	0.365	0.417	0.468	0.0151	0.111	1.10
COS	0.0118	0.0113	0.0133	0.0007	0.0036	0.031
N_2	17.31	17.75	16.97	26.19	33.22	23.39
CH_4	6.91	6.35	6.76	5.92	13.25	5.66
CO	18.85	18.98	18.89	23.15	25.56	2.89
C_6H_6	0.0875	0.0748	0.316	-----	-----	-----
C_7H_8	0.0849	0.0773	0.162	-----	-----	-----
Ethyl Benz.	N/A	N/A	N/A	N/A	N/A	N/A
Xylenes	N/A	N/A	N/A	N/A	N/A	N/A
Thiophene*	23	18	160	31	18	66
CH_3SH*	21	23	31	-----	1	23
C_2H_5SH*	-----	1	5	-----	1	7
CS_2*	3	3	20	1	1	5
Propylene*	1585	1255	1671	-----	384	168
Propane*	710	585	743	-----	218	444
Butane*	N/A	N/A	N/A	N/A	N/A	N/A
Methanol**	-----	-----	-----	-----	-----	3.15

*Parts per million (volume) **Estimated

TABLE D-6
GAS ANALYSIS SUMMARY FOR AMI-52/GO-72

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	31.82	31.96	31.31	42.81	21.97	0.00
CO_2	22.04	21.49	22.63	-----	11.37	62.96
C_2H_4	0.405	0.401	0.187	-----	-----	1.10
C_2H_6	0.545	0.544	0.257	-----	-----	1.59
H_2S	0.333	0.313	0.302	0.0105	0.0731	0.541
COS	0.0079	0.0065	0.0067	0.0006	0.0022	0.180
N_2	20.68	22.19	21.14	28.55	24.29	23.07
CH_4	6.23	5.73	6.04	5.63	14.84	4.75
CO	17.92	17.31	18.08	22.88	27.51	2.83
C_6H_6	0.1071	0.1224	0.9837	-----	-----	0.2657
C_7H_8	0.0283	0.0353	0.1434	-----	-----	-----
Ethyl Benz.	N/A	N/A	N/A	N/A	N/A	N/A
Xylenes	N/A	N/A	N/A	N/A	N/A	N/A
Thiophene*	33	27	63	-----	-----	44
CH_3SH*	13	13	10	1	3	9
C_2H_5SH*	-----	-----	-----	-----	-----	
CS_2*	3	2	2	1	-----	5
Propylene*	1721	1797	919	188	565	N/A
Propane*	585	734	393	248	362	N/A
Butane*	N/A	N/A	N/A	N/A	N/A	N/A
Methanol**	-----	-----	-----	-----	-----	3.15

*Parts per million (volume) **Estimated

TABLE D-7
GAS ANALYSIS SUMMARY FOR AMI-53/GO-73B

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	32.59	32.92	32.92	43.25	25.69	0.00
CO_2	22.36	22.30	22.13	-----	16.80	70.68
C_2H_4	0.493	0.508	0.450	0.212	0.715	1.27
C_2H_6	0.691	0.694	0.647	0.454	1.066	1.803
H_2S	0.138	0.165	0.171	0.1072	0.0601	0.413
COS	0.0062	0.0059	0.0060	0.0007	0.0027	0.016
N_2	20.79	20.81	21.12	27.63	25.86	24.10
CH_4	5.45	5.53	5.29	6.47	9.21	2.70
CO	17.46	17.04	17.24	22.63	22.00	2.31
C_6H_6	0.0594	0.0578	0.0366	-----	0.0590	0.0241
C_7H_8	0.0598	0.0592	-----	-----	-----	-----
Ethyl Benz.	N/A	N/A	N/A	N/A	N/A	N/A
Xylenes	N/A	N/A	N/A	N/A	N/A	N/A
Thiophene*	26	54	15	-----	-----	37
CH_3SH*	7	4	5	2	2	-----
C_2H_5SH*	-----	-----	-----	2	17	-----
CS_2	1	2	1	-----	1	-----
Propylene*	1640	1785	1621	186	771	3577
Propane*	230	264	229	341	339	2436
Butane*	N/A	N/A	N/A	N/A	N/A	N/A
Methanol**	-----	-----	-----	-----	-----	4.14

*Parts per million (volume)　　**Estimated

TABLE D-8
GAS ANALYSIS SUMMARY FOR AMI-57/GO-76

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	31.60	31.11	31.29	42.38	15.58	0.00
CO_2	23.51	23.91	21.98	-----	25.99	64.74
C_2H_4	0.52	0.53	0.56	0.0242	1.28	1.54
C_2H_6	0.72	0.72	0.76	0.0164	1.92	2.13
H_2S	0.250	0.284	0.287	0.0048	0.090	0.66
COS	0.0078	0.0076	0.0076	0.0001	0.0041	0.027
N_2	19.36	19.61	19.93	26.79	19.27	23.06
CH_4	6.56	6.46	6.57	7.54	14.20	2.36
CO	17.29	17.47	17.92	23.35	21.55	1.80
C_6H_6	0.087	0.097	0.234	TRACE	0.0031	0.15
C_7H_8	0.031	0.034	0.534	0.0054	0.0033	0.030
Ethyl Benz.	0.0016	0.0017	0.0450	-----	-----	-----
Xylenes	0.0080	0.0094	0.1557	-----	-----	-----
Thiophene*	44	44	127	-----	-----	-----
CH_3SH*	16	29	28	TRACE	5	TRACE
C_2H_5SH*	TRACE	-----	8	-----	-----	-----
CS_2*	TRACE	3	TRACE	TRACE	TRACE	TRACE
Propylene*	1505	1521	1811	107	995	4640
Propane*	208	198	253	301	172	2203
Butane*	185	150	143	54	91	71
Methanol**	-----	-----	-----	-----	-----	3.68

*Parts per million (volume) **Estimated

TABLE D-9
GAS ANALYSIS SUMMARY FOR AMI-59/GO-78

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	27.49	27.61	28.64	39.55	24.42	0.61
CO_2	21.88	22.75	24.49	0.41	15.32	60.10
C_2H_4	0.33	0.41	0.35	0.069	0.53	1.08
C_2H_6	0.46	0.46	0.45	0.014	0.64	1.22
H_2S	0.244	0.199	0.318	0.019	0.080	0.73
COS	0.0074	0.0038	0.0069	0.0004	0.0023	0.0186
N_2	30.21	28.64	27.69	38.09	34.14	26.34
CH_4	8.46	6.93	7.12	7.06	11.12	3.57
CO	11.94	12.63	12.05	15.75	16.24	2.29
C_6H_6	0.017	0.823	0.212	0.0009	0.0029	0.245
C_7H_8	0.0358	0.404	0.383	0.0022	0.0032	0.0322
Ethyl Benz.	N/A	0.0022	0.0060	———	———	———
Xylenes	N/A	0.0143	0.0400	———	———	———
Thiophene*	30	72	35	———	———	———
CH_3SH*	53	57	32	———	4	79
C_2H_5SH*	———	———	———	———	———	———
CS_2*	2	2	1	———	———	5
Propylene*	1194	1278	2535	172	452	2784
Propane*	489	512	628	213	167	683
Butane*	201	217	447	60	70	378
Methanol**	———	———	———	———	———	4.21

*Parts per million (volume)   **Estimated

TABLE D-10
GAS ANALYSIS SUMMARY FOR AMI-60/GO-79

Species	Sample Train	PCS Tank	Sour Gas	Sweet Gas	Flash Gas	Acid Gas
H_2	32.13	32.57	32.60	43.01	21.55	-----
CO_2	21.68	21.82	21.68	-----	27.16	63.82
C_2H_4	0.30	0.30	0.32	0.065	0.69	0.95
C_2H_6	0.33	0.33	0.36	0.081	0.82	1.03
H_2S	0.206	0.174	0.214	0.026	0.108	0.597
COS	0.0084	0.0078	0.0084	0.0019	0.0044	0.0233
N_2	21.33	20.62	20.71	27.62	24.40	24.71
CH_4	6.78	6.65	6.61	7.44	-----	2.60
CO	17.06	17.17	17.25	21.90	25.18	2.06
C_6H_6	N/A	0.0272	0.0391	-----	-----	0.0592
C_7H_8	N/A	0.0278	0.0393	-----	-----	-----
Ethyl Benz.	N/A	N/A	N/A	N/A	N/A	N/A
Xylenes	N/A	N/A	N/A	N/A	N/A	N/A
Thiophene*	99	97	83	-----	-----	13
CH_3SH*	37	29	35	-----	-----	26
C_2H_5SH*	1	1	2	-----	-----	65
CS_2	2	2	2	-----	1	5
Propylene*	925	940	1012	212	381	1053
Propane*	273	277	314	66	364	5004
Butane*	451	1730	224	-----	145	434
Methanol**	-----	-----	-----	-----	-----	3.49

*Parts per million (volume) **Estimated

APPENDIX E
AGRS MASS BALANCE RESULTS

NCSU DEPARTMENT OF CHEMICAL ENGINEERING
ACID GAS REMOVAL SYSTEM

RUN NUMBER A-M-43
INTEGRATED RUN
DATE 11/19/1980

STREAM COMPOSITION (MOL %)

	SOUR GAS	SWEET GAS	FLASH GAS	STRIP N2	ACID GAS	* ABSORB EXIT	* FLASH EXIT	* STRIP EXIT
CO2	20.050	0.000	50.580	0.000	68.370	5.331	4.837	0.000
H2S	0.295	0.022	0.254	0.000	0.890	0.074	0.072	0.002
COS	0.012	0.001	0.015	0.000	0.032	0.003	0.003	0.000
MEOH	0.000	0.000	0.000	0.000	1.100	93.754	94.671	99.838
H2	32.420	43.400	9.390	0.000	0.000	0.000	0.000	0.000
CO	21.230	25.790	14.810	0.000	0.080	0.283	0.125	0.126
N2	18.700	23.010	9.080	100.000	28.210	0.188	0.092	0.000
CH4	6.590	7.530	10.640	0.000	0.520	0.187	0.073	0.034
C2H4	0.308	0.062	2.054	0.000	0.621	0.069	0.048	0.000
C2H6	0.508	0.112	3.083	0.000	1.020	0.112	0.079	0.000

* CALCULATED

MASS BALANCE (LB-MOLES/HR)

	IN		OUT					
	SOUR GAS	STRIP N2	SWEET GAS	FLASH GAS	ACID GAS	* TOTAL IN	* TOTAL OUT	PERCENT RECOVERY
CO2	0.506	0.000	0.000	0.051	0.506	0.506	0.558	110.20
H2S	0.007	0.000	0.000	0.000	0.007	0.007	0.007	97.79
COS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	91.19
MEOH	0.000	0.000	0.000	0.000	0.008	0.000	0.000	0.00
H2	0.818	0.000	0.856	0.010	0.000	0.818	0.866	105.85
CO	0.536	0.000	0.509	0.015	0.001	0.536	0.525	97.91
N2	0.472	0.182	0.454	0.009	0.209	0.654	0.672	102.76
CH4	0.166	0.000	0.149	0.011	0.004	0.166	0.163	98.16
C2H4	0.008	0.000	0.001	0.002	0.005	0.008	0.008	101.64
C2H6	0.013	0.000	0.002	0.003	0.008	0.013	0.013	100.61
TOTAL (LB-MOLES/HR)	2.523	0.182	1.973	0.102	0.740	2.708	2.812	103.8

* METHANOL-FREE BASIS

TOTAL METHANOL LOSS = 0.008 LB-MOLES/HR = 0.038 GALLONS/HR

NCSU DEPARTMENT OF CHEMICAL ENGINEERING
ACID GAS REMOVAL SYSTEM

RUN NUMBER A-M-44
INTEGRATED RUN
DATE 12/15/1980

STREAM COMPOSITION (MOL %)

	SOUR GAS	SWEET GAS	FLASH GAS	STRIP N2	ACID GAS	* ABSORB EXIT	* FLASH EXIT	* STRIP EXIT
CO2	22.200	1.290	34.280	0.000	62.410	5.457	5.380	0.000
H2S	0.290	0.028	0.180	0.000	0.700	0.069	0.069	0.007
COS	0.011	0.001	0.008	0.000	0.020	0.003	0.003	0.001
MEOH	0.000	0.000	0.000	0.000	0.000	94.056	94.283	99.992
H2	30.470	39.450	18.330	0.000	0.780	0.043	0.000	0.000
CO	14.260	18.340	13.640	0.000	0.940	0.044	0.008	0.000
N2	24.660	31.890	23.000	100.000	25.030	0.042	0.000	0.000
CH4	7.250	8.600	9.250	0.000	1.590	0.166	0.142	0.000
C2H4	0.430	0.260	0.710	0.000	0.690	0.059	0.058	0.000
C2H6	0.490	0.330	0.790	0.000	0.730	0.061	0.059	0.000

* CALCULATED

MASS BALANCE (LB-MOLES/HR)

	IN		OUT					
	SOUR GAS	STRIP N2	SWEET GAS	FLASH GAS	ACID GAS	* TOTAL IN	* TOTAL OUT	PERCENT RECOVERY
CO2	0.540	0.000	0.024	0.009	0.524	0.540	0.556	103.01
H2S	0.007	0.000	0.001	0.000	0.006	0.007	0.006	91.30
COS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	69.21
MEOH	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.00
H2	0.741	0.000	0.737	0.005	0.007	0.741	0.748	100.96
CO	0.347	0.000	0.343	0.003	0.008	0.347	0.354	102.05
N2	0.600	0.182	0.596	0.006	0.210	0.782	0.812	103.79
CH4	0.176	0.000	0.161	0.002	0.013	0.176	0.176	99.99
C2H4	0.010	0.000	0.005	0.000	0.006	0.010	0.011	103.49
C2H6	0.012	0.000	0.006	0.000	0.006	0.012	0.012	104.77
TOTAL (LB-MOLES/HR)	2.433	0.182	1.869	0.025	0.839	2.617	2.677	102.3

* METHANOL-FREE BASIS

TOTAL METHANOL LOSS = 0.000 LB-MOLES/HR = 0.000 GALLONS/HR

NCSU DEPARTMENT OF CHEMICAL ENGINEERING
ACID GAS REMOVAL SYSTEM

RUN NUMBER A-M-45
INTEGRATED RUN
DATE 1/15/1981

STREAM COMPOSITION (MOL %)

	SOUR GAS	SWEET GAS	FLASH GAS	STRIP N2	ACID GAS	* ABSORB EXIT	* FLASH EXIT	* STRIP EXIT
CO2	20.720	2.580	13.510	0.000	58.020	2.421	2.358	0.000
H2S	0.255	0.026	0.100	0.000	0.520	0.030	0.030	0.006
COS	0.008	0.000	0.003	0.000	0.023	0.001	0.001	0.000
MEOH	0.000	0.000	0.000	0.000	0.426	96.419	96.953	99.875
H2	31.120	40.900	19.310	0.000	0.510	0.224	0.115	0.094
CO	17.540	20.890	25.640	0.000	3.430	0.325	0.181	0.025
N2	21.490	27.930	24.110	100.000	27.270	0.183	0.047	0.000
CH4	6.030	5.280	13.380	0.000	5.040	0.287	0.212	0.000
C2H4	0.370	0.023	0.390	0.000	1.060	0.045	0.043	0.000
C2H6	0.520	0.037	0.620	0.000	1.600	0.063	0.060	0.000

* CALCULATED

MASS BALANCE (LB-MOLES/HR)

	IN		OUT					
	SOUR GAS	STRIP N2	SWEET GAS	FLASH GAS	ACID GAS	* TOTAL IN	* TOTAL OUT	PERCENT RECOVERY
CO2	0.489	0.000	0.044	0.014	0.485	0.489	0.543	111.03
H2S	0.006	0.000	0.000	0.000	0.004	0.006	0.005	81.30
COS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	109.39
MEOH	0.000	0.000	0.000	0.000	0.004	0.000	0.000	0.00
H2	0.735	0.000	0.694	0.020	0.004	0.735	0.718	97.72
CO	0.414	0.000	0.354	0.027	0.029	0.414	0.410	98.94
N2	0.507	0.182	0.474	0.025	0.228	0.690	0.727	105.42
CH4	0.142	0.000	0.090	0.014	0.042	0.142	0.146	102.32
C2H4	0.009	0.000	0.000	0.000	0.009	0.009	0.010	110.62
C2H6	0.012	0.000	0.001	0.001	0.013	0.012	0.015	119.39
TOTAL (LB-MOLES/HR)	2.361	0.182	1.696	0.105	0.837	2.497	2.573	103.0

* METHANOL-FREE BASIS

TOTAL METHANOL LOSS = 0.004 LB-MOLES/HR = 0.017 GALLONS/HR

NCSU DEPARTMENT OF CHEMICAL ENGINEERING
ACID GAS REMOVAL SYSTEM

RUN NUMBER A-M-47
INTEGRATED
DATE 1/27/1981

STREAM COMPOSITION (MOL %)

	SOUR GAS	SWEET GAS	FLASH GAS	STRIP N2	ACID GAS	* ABSORB EXIT	* FLASH EXIT	* STRIP EXIT
CO2	21.920	0.090	9.300	0.000	61.370	2.782	2.740	0.000
H2S	0.468	0.015	0.111	0.000	1.100	0.058	0.058	0.004
COS	0.013	0.001	0.004	0.000	0.031	0.002	0.002	0.000
MEOH	0.000	0.000	0.000	0.000	3.000	96.140	96.502	99.794
H2	34.040	44.990	17.680	0.000	0.000	0.266	0.168	0.174
CO	18.890	23.150	25.830	0.000	2.890	0.312	0.168	0.028
N2	16.970	26.190	33.670	100.000	23.390	0.000	0.000	0.000
CH4	6.760	5.920	13.250	0.000	5.660	0.325	0.252	0.000
C2H4	0.320	0.000	0.324	0.000	0.958	0.041	0.039	0.000
C2H6	0.583	0.000	0.606	0.000	1.666	0.074	0.071	0.000

* CALCULATED

MASS BALANCE (LB-MOLES/HR)

	IN		OUT					
	SOUR GAS	STRIP N2	SWEET GAS	FLASH GAS	ACID GAS	* TOTAL IN	* TOTAL OUT	PERCENT RECOVERY
CO2	0.521	0.000	0.002	0.010	0.558	0.521	0.569	109.18
H2S	0.011	0.000	0.000	0.000	0.010	0.011	0.010	93.11
COS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	93.74
MEOH	0.000	0.000	0.000	0.000	0.027	0.000	0.000	0.00
H2	0.810	0.000	0.760	0.018	0.000	0.810	0.778	96.14
CO	0.449	0.000	0.391	0.027	0.026	0.449	0.444	98.89
N2	0.404	0.182	0.442	0.035	0.213	0.586	0.690	117.82
CH4	0.161	0.000	0.100	0.014	0.051	0.161	0.165	102.81
C2H4	0.008	0.000	0.000	0.000	0.009	0.008	0.009	119.03
C2H6	0.014	0.000	0.000	0.001	0.015	0.014	0.016	113.90
TOTAL (LB-MOLES/HR)	2.378	0.182	1.689	0.105	0.909	2.559	2.683	104.8

* METHANOL-FREE BASIS

TOTAL METHANOL LOSS = 0.027 LB-MOLES/HR = 0.130 GALLONS/HR

NCSU DEPARTMENT OF CHEMICAL ENGINEERING
ACID GAS REMOVAL SYSTEM

RUN NUMBER A-M-52
INTEGRATED
DATE 2/19/1981

STREAM COMPOSITION (MOL %)

	SOUR GAS	SWEET GAS	FLASH GAS	STRIP N2	ACID GAS	* ABSORB EXIT	* FLASH EXIT	* STRIP EXIT
CO2	22.630	0.000	11.370	0.000	62.960	2.891	2.844	0.000
H2S	0.302	0.010	0.073	0.000	0.541	0.038	0.037	0.012
COS	0.007	0.001	0.002	0.000	0.018	0.001	0.001	0.000
MEOH	0.000	0.000	0.000	0.000	3.150	96.004	96.534	99.893
H2	31.310	42.810	21.970	0.000	0.000	0.212	0.092	0.096
CO	18.080	22.880	27.510	0.000	2.830	0.285	0.135	0.000
N2	21.140	28.550	24.290	100.000	23.070	0.175	0.042	0.000
CH4	6.040	5.630	14.840	0.000	4.750	0.273	0.193	0.000
C2H4	0.405	0.000	0.000	0.000	1.095	0.052	0.052	0.000
C2H6	0.544	0.000	0.000	0.000	1.588	0.069	0.070	0.000

* CALCULATED

MASS BALANCE (LB-MOLES/HR)

	IN		OUT					
	SOUR GAS	STRIP N2	SWEET GAS	FLASH GAS	ACID GAS	* TOTAL IN	* TOTAL OUT	PERCENT RECOVERY
CO2	0.530	0.000	0.000	0.011	0.551	0.530	0.563	106.28
H2S	0.007	0.000	0.000	0.000	0.005	0.007	0.005	70.43
COS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	108.16
MEOH	0.000	0.000	0.000	0.000	0.028	0.000	0.000	0.00
H2	0.733	0.000	0.694	0.022	0.000	0.733	0.716	97.71
CO	0.423	0.000	0.371	0.028	0.025	0.423	0.423	100.04
N2	0.495	0.182	0.463	0.024	0.202	0.677	0.689	101.82
CH4	0.141	0.000	0.091	0.015	0.042	0.141	0.148	104.54
C2H4	0.009	0.000	0.000	0.000	0.010	0.009	0.010	101.24
C2H6	0.013	0.000	0.000	0.000	0.014	0.013	0.014	109.25
TOTAL (LB-MOLES/HR)	2.341	0.182	1.621	0.101	0.876	2.533	2.568	101.4

* METHANOL-FREE BASIS

TOTAL METHANOL LOSS = 0.028 LB-MOLES/HR = 0.132 GALLONS/HR

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                    NCSU DEPARTMENT OF CHEMICAL ENGINEERING
                       ACID   GAS   REMOVAL   SYSTEM

                           RUN NUMBER A-M-53
                            INTEGRATED
                           DATE    3/12/1981


                         STREAM COMPOSITION (MOL %)
                         ------ -----------
                                                              *         *         *
            SOUR     SWEET     FLASH     STRIP     ACID     ABSORB     FLASH     STRIP
            GAS      GAS       GAS       N2        GAS      EXIT       EXIT      EXIT

 CO2       22.130    0.000    16.490     0.000    65.280     3.026     3.002     0.000
 H2S        0.171    0.017     0.060     0.000     0.413     0.022     0.022     0.001
 COS        0.006    0.001     0.003     0.000     0.016     0.001     0.001     0.000
 MEOH       0.000    0.000     0.000     0.000     4.140    96.591    96.761    99.976
 H2        32.920   43.250    25.220     0.000     0.000     0.066     0.021     0.022
 CO        17.240   22.630    22.000     0.000     2.310     0.037     0.000     0.000
 N2        21.120   27.630    25.390   100.000    22.250     0.055     0.009     0.000
 CH4        5.290    6.470     9.040     0.000     2.490     0.060     0.044     0.000
 C2H4       0.450    0.021     0.715     0.000     1.270     0.059     0.058     0.000
 C2H6       0.647    0.045     1.066     0.000     1.803     0.084     0.082     0.000

                                                        * CALCULATED


                         MASS BALANCE (LB-MOLES/HR)
                         ---- -------

                 IN                      OUT
            -------------       -------------------         *        *
            SOUR     STRIP     SWEET     FLASH     ACID     TOTAL     TOTAL   PERCENT
            GAS      N2        GAS       GAS       GAS      IN        OUT     RECOVERY

 CO2        0.551    0.000     0.000     0.005     0.581    0.551     0.586    106.34
 H2S        0.004    0.000     0.000     0.000     0.004    0.004     0.004     94.33
 COS        0.000    0.000     0.000     0.000     0.000    0.000     0.000    105.18
 MEOH       0.000    0.000     0.000     0.000     0.037    0.000     0.000      0.00
 H2         0.820    0.000     0.808     0.008     0.000    0.820     0.816     99.52
 CO         0.429    0.000     0.423     0.007     0.021    0.429     0.450    104.89
 N2         0.526    0.182     0.516     0.008     0.198    0.708     0.722    101.99
 CH4        0.132    0.000     0.121     0.003     0.022    0.132     0.146    110.76
 C2H4       0.011    0.000     0.000     0.000     0.011    0.011     0.012    106.48
 C2H6       0.016    0.000     0.001     0.000     0.016    0.016     0.017    106.95

 TOTAL      2.491    0.182     1.868     0.032     0.890    2.672     2.754    103.1
 (LB-MOLES/HR)
                                                   * METHANOL-FREE BASIS

        TOTAL METHANOL LOSS =  0.037 LB-MOLES/HR =  0.176 GALLONS/HR
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NCSU DEPARTMENT OF CHEMICAL ENGINEERING
ACID GAS REMOVAL SYSTEM

RUN NUMBER A-M-57
INTEGRATED RUN
DATE 4/28/1981

STREAM COMPOSITION (MOL %)

	SOUR GAS	SWEET GAS	FLASH GAS	STRIP N2	ACID GAS	* ABSORB EXIT	* FLASH EXIT	* STRIP EXIT
CO2	21.980	0.000	25.990	0.000	64.740	5.086	4.923	0.245
H2S	0.287	0.003	0.090	0.000	0.660	0.066	0.065	0.019
COS	0.008	0.000	0.004	0.000	0.027	0.002	0.002	0.000
MEOH	0.000	0.000	0.000	0.000	3.130	94.085	94.611	99.553
H2	31.790	42.380	15.680	0.000	0.000	0.083	0.000	0.000
CO	17.920	23.350	21.550	0.000	1.800	0.140	0.000	0.000
N2	19.930	26.790	19.270	100.000	23.060	0.014	0.000	0.174
CH4	6.570	7.540	14.200	0.000	2.360	0.226	0.123	0.000
C2H4	0.558	0.024	1.282	0.000	1.537	0.125	0.116	0.005
C2H6	0.759	0.016	1.922	0.000	2.135	0.173	0.160	0.005

* CALCULATED

MASS BALANCE (LB-MOLES/HR)

	IN		OUT					
	SOUR GAS	STRIP N2	SWEET GAS	FLASH GAS	ACID GAS	* TOTAL IN	* TOTAL OUT	PERCENT RECOVERY
CO2	0.475	0.000	0.000	0.018	0.435	0.475	0.453	95.46
H2S	0.006	0.000	0.000	0.000	0.004	0.006	0.005	73.57
COS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	109.46
MEOH	0.000	0.000	0.000	0.000	0.021	0.000	0.000	0.00
H2	0.687	0.000	0.679	0.011	0.000	0.687	0.689	100.42
CO	0.387	0.000	0.374	0.015	0.012	0.387	0.401	103.56
N2	0.430	0.182	0.429	0.013	0.155	0.613	0.597	97.51
CH4	0.142	0.000	0.121	0.010	0.016	0.142	0.146	103.12
C2H4	0.012	0.000	0.000	0.001	0.010	0.012	0.012	96.30
C2H6	0.016	0.000	0.000	0.001	0.014	0.016	0.016	97.21
TOTAL (LB-MOLES/HR)	2.160	0.182	1.602	0.068	0.673	2.338	2.319	99.2

* METHANOL-FREE BASIS

TOTAL METHANOL LOSS = 0.021 LB-MOLES/HR = 0.101 GALLONS/HR

NCSU DEPARTMENT OF CHEMICAL ENGINEERING
ACID GAS REMOVAL SYSTEM

RUN NUMBER A-M-59
INTEGRATED RUN
DATE 5/25/1981

STREAM COMPOSITION (MOL %)

	SOUR GAS	SWEET GAS	FLASH GAS	STRIP N2	ACID GAS	* ABSORB EXIT	* FLASH EXIT	* STRIP EXIT
CO2	22.750	0.410	15.320	0.000	60.100	2.564	2.537	0.075
H2S	0.318	0.019	0.080	0.000	0.730	0.035	0.035	0.005
COS	0.007	0.000	0.002	0.000	0.018	0.001	0.001	0.000
MEOH	0.000	0.000	0.000	0.000	4.210	96.970	97.063	99.885
H2	27.610	39.550	24.420	0.000	0.610	0.000	0.000	0.000
CO	12.630	15.250	16.240	0.000	2.290	0.138	0.108	0.014
N2	28.640	38.090	34.140	100.000	26.340	0.013	0.000	0.000
CH4	6.930	7.060	11.120	0.000	3.570	0.188	0.167	0.021
C2H4	0.408	0.069	0.530	0.000	1.080	0.041	0.040	0.000
C2H6	0.460	0.014	0.640	0.000	1.220	0.051	0.050	0.000

* CALCULATED

MASS BALANCE (LB-MOLES/HR)

	IN		OUT					
	SOUR GAS	STRIP N2	SWEET GAS	FLASH GAS	ACID GAS	* TOTAL IN	* TOTAL OUT	PERCENT RECOVERY
CO2	0.471	0.000	0.006	0.005	0.447	0.471	0.458	97.21
H2S	0.007	0.000	0.000	0.000	0.005	0.007	0.006	87.22
COS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	96.89
MEOH	0.000	0.000	0.000	0.000	0.031	0.000	0.000	0.00
H2	0.572	0.000	0.614	0.008	0.005	0.572	0.627	109.53
CO	0.262	0.000	0.237	0.006	0.017	0.262	0.259	99.05
N2	0.593	0.199	0.591	0.012	0.196	0.792	0.798	100.78
CH4	0.144	0.000	0.110	0.004	0.027	0.144	0.140	97.42
C2H4	0.008	0.000	0.001	0.000	0.008	0.008	0.009	109.75
C2H6	0.010	0.000	0.000	0.000	0.009	0.010	0.010	99.70
TOTAL (LB-MOLES/HR)	2.072	0.199	1.552	0.034	0.743	2.266	2.307	101.8

* METHANOL-FREE BASIS

TOTAL METHANOL LOSS = 0.031 LB-MOLES/HR = 0.149 GALLONS/HR